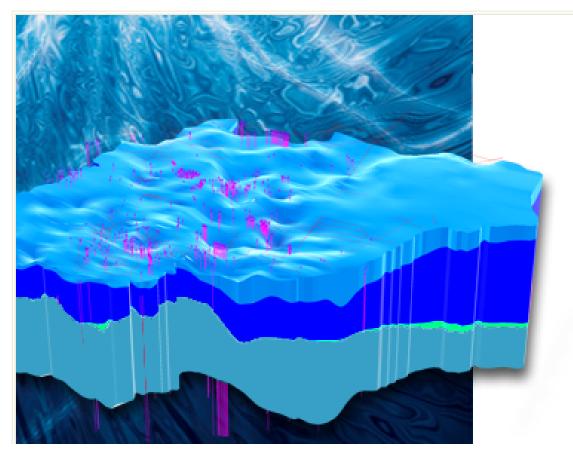
User's Manual



Visual MODFLOW Flex 9.0

Integrated Conceptual & Numerical Groundwater Modeling Software

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1 Introduction

Visual MODFLOW (VMOD) Flex is a powerful software package that provides the tools for building three-dimensional groundwater conceptual and numerical models using raw GIS data objects. The conceptual model approach to groundwater modeling allows you to:

- Build a conceptual model of the groundwater system, prior to the simulation Geologic formation structures, hydrogeologic properties, and boundary conditions are all designed outside the model grid or mesh; this allows the flexibility to adjust your interpretation of the groundwater system before applying a discretization method and converting to a numerical model.
- Build the model with minimal data pre-processing required Working with gridindependent data allows you to maximize the use of your existing GIS data and incorporate physical geology and geographic conditions before designing a grid or mesh.
- Generate and simulate regional and local-scaled models With support for MODFLOW-LGR, you can design local grids around areas of interest, directly within the conceptual model environment. Calculated heads from a regional model can also be used as boundary conditions for local-scaled models.
- Design the correct model faster The grid-independent raw data is left intact and is not constricted by grid cells or mesh elements when modifying the data and project objective. This allows you to generate multiple numerical models from the same conceptual model.
- *Make changes to the model data and immediately see results* The conceptual model environment provides simultaneous 2D and 3D views which are updated whenever changes to the data are made.

This document provides detailed descriptions of all features and functionality available in Visual MODFLOW Flex.

How to get started
Study this Introduction chapter and Program Overview sections to familiarize yourself with the program.
Then work through the <u>Quick Start Tutorials</u> to familiarize yourself with using VMOD Flex. These sections cover importing MODFLOW and VMOD Classic projects as well as building new models using the Conceptual Modeling approach.

Learning more

- See <u>Conceptual Modeling Workflow</u> for instructions on building a grid-independent conceptual model using your raw data
- See <u>Numerical Modeling Workflow</u> for more instructions on working with numerical inputs, translating to MODFLOW packages, and running and analyzing the results.
- See <u>Working with Multiple Model Scenarios</u> for a better understanding of the various workflows in VMOD Flex.
- See the <u>Program Overview</u> section for detailed instructions on using VMOD Flex.
- Looking for help beyond what's in this manual? We have many additional resources for you:
 - ✓ Getting Started with Visual MODFLOW Flex
 - ✓ An Introduction to Groundwater Modeling Concepts
 - ✓ LinkedIn User's Group
 - ✓ <u>Visual MODFLOW Flex Frequently Asked Questions</u> (FAQ)
 - ✓ Your Complete Guide to MODFLOW-USG
 - ✓ <u>All Tutorials</u>
 - ✓ Visual MODFLOW Flex ReadMe
 - ✓ White Papers & Technical Articles

1.1 Installation and Licensing

Hardware Requirements

To run the latest version of **Visual MODFLOW Flex**, you will need the following minimum system configuration:

	Windows 10 (Pro, Enterprise, or Ultimate)
Operating System	Windows 11 (Pro, Enterprise, or Ultimate)
	NOTE: Administrative rights may be required to install the software
Processor	32-bit or 64-bit (Pentium 4 or higher)
RAM	8GB or more recommended*
Hard Disk	1.5 GB Free Space, plus extra space for your models
Networking Hardware	Network Card (required for soft key licensing)
Software	MS-Office (2000 or later). If you do not have Office, you must install the Access Database Engine

* If you intend to work with larger models, it is recommended that you use 64-bit version of Visual MODFLOW Flex and increase your RAM above the minimum requirements. The following table of model size (number of cells vs. stress periods) shows recommendations for memory size based on a simple benchmark model using a dedicated computer (i.e. no other active applications). Results will vary depending on several factors including the number and complexity of boundary conditions and property zones.

		Total Number of Model Cells							
		<1M	1M	2M	3M	4M	5M	6M	6M+
	<10	8Gb	8Gb	12Gb	12Gb	16Gb	16Gb	32Gb	32Gb
Stress Periods	50	8Gb	12Gb	12Gb	16Gb	16Gb	32Gb	32Gb	64Gb
50033101003	100	12Gb	12Gb	16Gb	16Gb	32Gb	32Gb	32Gb	64Gb
	100+	12Gb	16Gb	16Gb	32Gb	32Gb	64Gb	64Gb	NR

M = million NR= not recommended

Software Requirements

To run the latest version of Visual MODFLOW Flex, the following software pre-requisites are required:

Microsoft .NET Framework v.4.0 installed (provided with installation)

Microsoft Office 2000 (or later) or Microsoft Access Database Engine

NOTE: Microsoft Office 64-bit version is currently not supported for XLS and MDB import.

If you have any problems with your particular system configuration, please contact your system administrator, or technical support: support@waterloohydrogeologic.com

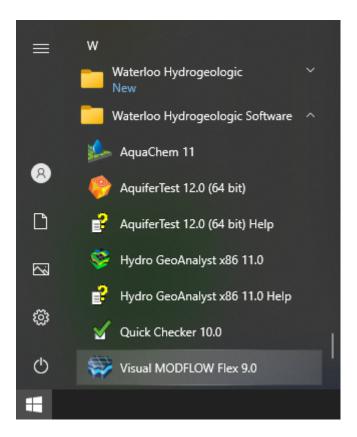
Installation and Licensing

When you purchase Visual MODFLOW Flex, you will receive download and installation instructions. Please consult these for the latest instructions.

Please Note: If you are using dongle-based hardware licensing, please ensure that your dongle is connected to your computer AFTER you have installed the software, and that you have properly configured your installation.

Starting Visual MODFLOW Flex

Once Visual MODFLOW Flex has been installed on your computer, simply double-click on the Visual MODFLOW Flex shortcut icon () located on your computer's desktop. Alternatively, you can access the software via the Start Menu by clicking on the Windows button and looking under the Waterloo Hydrogeologic folder.



1.2 Features

Visual MODFLOW Flex is a graphical user interface for developing, running, and visualizing groundwater simulations that brings together industry-standard codes for groundwater flow and contaminant transport, essential analysis and calibration tools, and stunning 3D visualization capabilities in a single, easy-to use software environment.

Work With Geographic Data

Visual MODFLOW Flex supports the following coordinate systems:

- Geographic coordinate systems (data import only)
- Projected coordinate systems: UTM, State Plane
- Local Cartesian

Work With Grid-Independent Data

Import spatial and attribute data from a wide variety of data types including:

- Points (.XLSX, .TXT, .CSV, .MDB, .SHP, .DXF, .TRP)
- Polylines (.SHP, .DXF)
- Polygons (.SHP, .DXF)
- 3D Gridded Data (.HDS, .DAT, .UCN)

- Raster Images (.BMP, .TIF, .JPG)
- Time Schedules (.XLSX)
- Surfaces (.DEM, .GRD, .TXT. ,.ASC)
- Hydro GeoAnalyst (HGA) Cross Sections (.3XS)
- Vertical and Non-vertical Wells (.XLSX, .CSV)

View and modify settings for imported data:

- View data object meta data including the source file name, field mappings and the native coordinate system
- View raw attribute data in a spreadsheet view
- Apply mathematical operations to data, e.g., set an attribute as a constant value, convert well tops to a points data object, and convert HGA cross section model layers to a points data object
- Drape a raster image over a surface data object, e.g., digital elevation models
- Set symbol properties for points, polygons, polylines and display labels using a variety of style options
- Color render shape features by attribute value using a classified or stretched color scheme
- Show contour lines and set color rendering options for surface layers
- Add, remove and modify wells and associated well data including screens intervals, diver observation points, well tops, well paths (for horizontal only), and pumping schedules

Create surfaces from points data objects:

- Using one or more point data objects, generate surface layers using Inverse Distance, Kriging, or Natural Neighbor interpolation methods
- Configure the interpolation method by modifying various interpolation settings
- Clip the generated surface to the horizontal extents of a specified polygon data object

Digitize new data objects using 2D Viewer:

 Using the 2D Viewer editing tools, digitize a new point, polyline, polygon, or well data object

2D & 3D Visualization

Visualize data objects and conceptual model features using interactive 2D and 3D Viewers:

- Use various screen configurations to display multiple 3D or 2D Viewers simultaneously
- Zoom, rotate, and move data within the viewer using your mouse or keyboard
- Modify viewer settings including the background color and vertical exaggeration (cross-section and 3D Viewers)
- In 3D Viewers, remove parts of the displayed data by creating cutaways along the X-, Y-, and Z-axes
- In 2D Viewers, select individual data object features (points, line, shapes) and then view the corresponding attribute data in spreadsheet view and vice versa

Edit data object geometry in 2D Viewer:

- Modify existing data objects by manually digitizing points, polylines, and polygons
- Rotate, scale, and delete shapes
- "Undo" all edits and revert back to original shape

Define Multiple Conceptual Models

Create multiple conceptual models:

- Create multiple conceptual models with different interpretations or copy existing conceptual models
- · Define conceptual model geometry using imported data objects
- Define the horizontal model boundary using an imported or digitized polygon data object
- Create vertical horizons from surfaces that are either imported or created by interpolating raw XYZ points
- Select from different horizon types to accommodate various geological conditions (pinchouts, discontinuous layers, etc.)
- Automatically create 3D structural zones from defined horizons

Property Modeling

- Create property zones from imported polygon data objects, digitized polygon data objects, or generated structural zones
- Assign property values for conductivity, storage, and initial heads using various data sources:
 - o a constant value
 - o imported polygon shapefile attributes
 - o imported 3D gridded data attributes
 - o surface data objects

Boundary Condition Modeling

Create Boundary Conditions

- Automatically generate the simulation domain using the boundaries defined for the conceptual model
- Apply boundary conditions to the top, bottom, sides or an intermediate layer of the simulation model domain
- Support for the following groundwater flow and transport boundary conditions:
 - Drain (DRN)
 - Evapotranspiration (EVT)
 - Flow and Head Boundary/Specified Flux (FHB)
 - General Head (GHB)
 - o Horizontal Flow Barrier/Wall (HFB)
 - o Lake (LAK)
 - Mass Source Loading (SCR) (MODFLOW-6 *only*)
 - Pumping Wells (WEL) and Multi-Node Pumping Wells (MNW1, MNW2)

- Recharge (RCH)
- Recharge Seepage Face (RSF) (MODFLOW-SURFACT only)
- Rivers and Streams (RIV, SFR)
- Specified Concentration (SSM, CNC)
- Specified Head (CHD)
- o Time Varying Material Properties (TMP) (MODFLOW-SURFACT only)
- Unsaturated Zone (UZF)
- For linear boundary conditions, define local zones from line segments using an interactive 2D Viewer window
- For linear boundary conditions, define parameters at starting, ending, or intermediate vertices along a line and interpolate values between each vertex
- Set each boundary condition parameter as static or transient
- Define boundary condition parameters using one or more of the following data sources:
 - o constant value
 - o imported shapefile attributes
 - o attributes from 3D Gridded data objects
 - o surface data objects
 - o time schedule data object (for transient boundary conditions)

Model Discretization

Discretize your model using finite-difference, finite-element, or control volume methods:

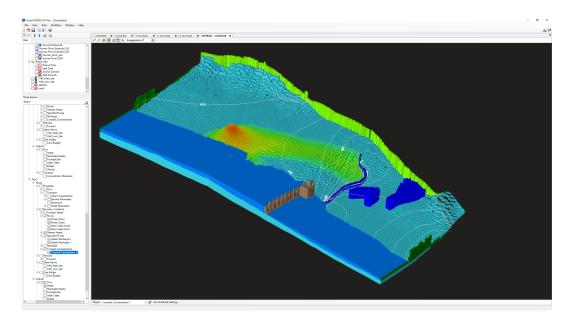
- When working with finite-difference grids:
 - o Specify the number of rows and columns, grid origin, and the angle of rotation
 - Choose from the following finite difference grid types: Deformed, Uniform, Semi-Uniform
 - Perform horizontal grid refinement/coarsening within a user-defined row/column interval
 - Define a child grid within a numerical grid for running Local Grid Refinement (LGR) simulations using the MODFLOW-LGR flow engine
- When working with finite-elements meshes:
 - o Use imported shape data objects to define the super-element mesh
 - Choose from various Delaunay triangulation methods including constrained and conforming
 - o Refine areas of the mesh using digitized or imported polygon shapes
 - o Fit the mesh to your model domain using deformed or semi-uniform vertical slices
- When working with unstructured grids:
 - Define unstructured Voronoi and/or Quad-tree grids based on imported and created grid-independent feature objects (see related section above)
 - $_{\odot}$ Refine areas of the grid around wells and boundary conditions
 - Accommodate pinchout layers when generating the numerical model, for accurate representation of complex geologic conditions

1.3 What's New

Version 9.0 - March 2023

MODFLOW-6 Groundwater Flow and Transport

Visual MODFLOW Flex now supports <u>MODFLOW-6</u>, the newest core version of the groundwater modeling code developed by the USGS. MODFLOW-6 is based on a redesigned framework that supports 3D groundwater flow, solute transport, and various processes with an all new and more legible input file structure for both structured and unstructured grids.



The following MODFLOW-6 flow packages are supported in Visual MODFLOW Flex:

- Simulation Packages:
 - o MFSIM.NAM Simulation Name File
 - o TDIS Time Discretization
 - o IMS Iterative Model Solution
- Groundwater Flow Model (GWF): Simulate saturated groundwater flow using structured finite difference grids or unstructured control volume finite difference grids (Voronoi or Quadtree).
 - o GWF.NAM Groundwater Flow Model Name File
 - o DIS Discretization Package
 - o DISV Discretization by Vertices Package
 - IC Initial Conditions (Heads)
 - **OC** Output Control Package
 - NPF Node Property Flow Package
 - **STO** Storage Package
 - CHD* Time Varying Constant Head Package

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- WEL* Well Package
- DRN* Drain Package
- RIV* River Package
- o GHB* General-Head Boundary Package
- o RCH Recharge Package
- o EVT Evapotranspiration Package
- Solute Transport Model (GWT): Simulate groundwater solute transport using structured finite difference grids or unstructured control volume finite difference grids (Voronoi or Quadtree), including a variety of sorption, reaction, and immobile domain models.
 - o GWT.NAM Groundwater Transport Model Name File
 - o DIS Discretization Package
 - o **DISV** Discretization by Vertices Package
 - o IC Initial Conditions (Concentrations)
 - o OC Output Control Package
 - ADV Advection Package
 - o **DSP** Dispersion Package
 - o MST Mobile Storage Transfer Package
 - o **IST** Immobile Storage Transfer Package (up to three immobile domains)
 - o SSM Source Sink Mixing Package
 - CNC* Time Varying Constant Concentration Package
 - SRC* Mass Source Loading Package
- **Multiple Instance Packages**: MODFLOW-6 allows you to include multiple instances of certain packages (marked with * above) in a simulation and track budgets separately for each package.
- Support for ZoneBudget-6: Evaluate sub-regional flows for your groundwater flow models using MODFLOW-6.

Engines and Packages

- Assign Grid (In)active cell zones using data objects: You can use point, polyline, and polygon data objects to set the active/inactive flag for grid cells in the Finite Difference grid workflows
- Import MNW1 Wells from Classic Projects: Well information using the MNW1 well model in Classic Projects can be imported into Visual MODFLOW Flex
- Minimum thickness for Unstructured Grids: You can specify a minimum cell thickness below which unstructured grid cells will be removed from the grid so that you have more control on grid design around pinchout areas.
- MODPATH with SEAWAT: You can run a MODPATH particle tracking simulation based on a SEAWAT flow (and transport) run.
- **Compare**: Compare results for heads, drawdowns, or concentrations between two model runs using the same unstructured grid.

Performance, Usability, and Other Enhancements

- The unstructured grid workflow now uses the more familiar and intuitive conceptual well controls that uses coordinates and well screen information instead of cell indices
- You can specify default Total and Effective Porosity values at the Define Modeling Objectives step
- You can add particles for a particle track simulation based on Well objects in the Model Explorer as well as in the Data Explorer
- · Improved speed and performance saving and loading projects
- You can specify a custom default project save location to save time when creating new projects
- New Keyboard Shortcuts:

 Press CTRL+T at the Translate Step to translate a model
 Press CTRL+R at the Run Step to run a model

Defects Addressed

- Unhandled exception when replacing layer elevations with a surface containing holes (NoData) values
- Contour lines not shown for intervals with high precision/very small increments in some cases
- Intermittent "Failed to apply settings" error when visualizing recharge or evapotranspiration rates in some views
- Some view style settings do not honor the "Show in Cutaway" option
- In some cases, boundary condition schedules are not translated correctly in the SSM package
- Various windows issues with high resolution monitors:
 - Expression Builder window
 - o Create Surface/Interpolation Settings window
 - o Editing Conceptual Boundary Conditions
- o Define Property Zones step in the Conceptual Workflow
- In some cases, pathlines would not be exported as a shapefile
- Error editing numerical boundary condition in some cases
- Unhandled "index was out of range" error while copying property zones to another model property
- Error using the fill buttons on the Active checkbox field in the Edit Boundary Condition window
- Can't save lake gauge data when there are no streams in the SFR workflow
- Errors realizing lakes using SFR workflow without streams
- In some cases, importing concentrations via a UCN file resets inactive cell flag to active in the associated grid where the water table is below grid layer 1
- Error creating boundary condition using a surface as a data source in some cases
- · Error importing well schedule using absolute date with certain formats

- Editing the recharge database did not always edit the recharge boundary condition
- Transient Model with Steady-State stress period does not translate correctly
- Unable to run MODPATH due to null reference error
- Calibration Dashboard did not correctly report units in the summary statistics based on the selection
- Issue with defining boundary conditions for certain shapefiles
- Issue running PEST in some situations when parameter zones do not extend through all model layers
- Failed to move to target step error of Surface Water Workflow in some conceptual models
- Errors creating variograms in the PEST workflow in some cases
- Particle tracking pathlines do not display correct units/values due to unit conversion errors for some combinations of project units
- Unable to translate MNW2 package under some circumstances
- When draping basemap images onto a surface using the operations, only a limited number of points were sampled

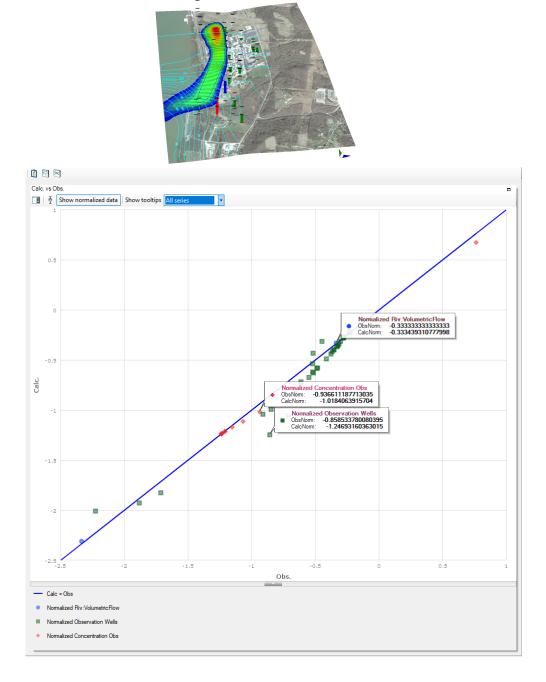
For full version history, see the Visual MODFLOW Flex readme file at: https://www.waterloohydrogeologic.com/visual-modflow-flex-readme/

1.3.1 Version 8.0

Calibration and Observations

Support for the following observation types:

- Wells/Points: head, concentration
- Boundary Condition Flow: net volumetric flow exchange between groundwater and a specified boundary condition
- ZoneBudget Zone Flow: net volumetric flow exchange of groundwater in/out of a specified zone, between a specified zone and another zone or a specified boundary condition type
- Surface Water gages:
 - Stream (SFR): stage, depth, outflow, head difference between stream midpoint and associated groundwater cell centroid, flow diverted (diversion segments only), groundwater head, streambed seepage through the unsaturated zone
 - $\,\circ\,$ Lakes (LAK): stage, volume, inflow, outflow
- Import and/or set target residuals for observations



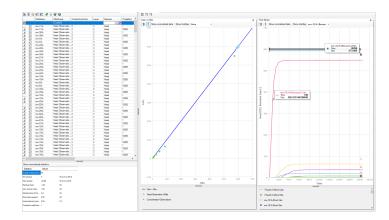
Calibration and Run Result Visualization

View model results using a dashboard to facilitate model calibration and results interpretation:

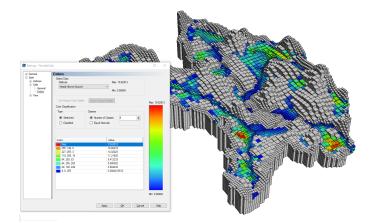
- Model Dashboard: model observations and associated model results can be displayed in the new model results dashboard which includes dynamic tabulation and charting of results:
 - Tabulated results: observations and corresponding simulated results are presented in a tabular format with dynamic filtering. Tabulated observations

include observation metadata, including time, location, observation group/type, model layer, and conductivity zone, so that you can quickly display all the data or limit the view to what is relevant.

- o Charts: simultaneously display one or more charts including:
 - simulated vs observed values to evaluate model calibration/history matching
 - time series to display and evaluate transient result



- Text Outputs: all observations and associated simulated results are output as tab separated variable text files for use in both Visual MODFLOW Flex and in external applications.
- Flooded Cells: Display cells with simulated heads above the top of the model as a flood depth map or as a solid color to facilitate model calibration and interpretation:



- Easily switch the location of subviews in a Flex Viewers so that you can customize the layout.
- Save and reload standalone 2D and 3D viewers
- Proportionally sized calibration residuals can be viewed for unstructured grid model runs

Packages and Model Runs

- **Single Engine Runs**: run a secondary model such as transport, particle track, or zone budget simulation without having to rerun your flow model.
- Update Solvers: update your flow model solvers without having to retranslate your whole model
- **Copy Property Zones**: copy/paste zones from one material property zone type to another so that you can more easily have consistent material zones across property types such as conductivity, storage, and transport parameters
- Default SMS Settings: the default settings for the SMS solver package in MODFLOW-USG have been updated based on recommendations by the author of MODFLOW-USG
- **Gage Package**: gage package is supported in models using the surface water network workflows for streams (SFR) and lakes (LAK).

Surface Water Workflow

- **Conceptual Workflow**: Build surface water stream and lake networks in a conceptual model and convert it to numerical models
- Clone Workflow: surface water workflows are copied into applicable runs when editing a grid or cloning a model run

Data Handling

- **Data Operations**: data objects use the expression builder, facilitating greater control and flexibility when adjusting data object elevations for surfaces, points, polylines, and polygons.
- Expression Builder functions: added a function called ifgaps() to handle expressions with non-overlapping surfaces now you can combine surfaces with different extents/scales such as regional and site surfaces using a single expression.
- Horizons: are now treated the same as other surfaces: they can be shown in 2D views with control over display settings
- Cell Inspector Feedback: Typing a cell ID in the cell inspector provides (optional) feedback on where the specified cell is located in the active view
- Export more data objects:
 - o Grids: shapefile,
 - o Output Comparisons: shapefile, contours, and surface
 - o Horizons: surface
 - Water Table: surface

Performance, Usability, and Other Enhancements

- Improved speed and performance for the following:
 - o Loading and editing model properties and boundary conditions in larger models
 - o Conceptual Model conversion to numerical models using unstructured Q-Grids
 - o Using the Cell inspector
 - o Model Translation
- Greater control over your project modeling data:
- Backup your project and related files as a zip file from the Main Menu to archive your project or easily share it with colleagues.

Backup Project	x
Backup name C:\Users\Public\Documents\Visual MODFLOW Flex\Projects\project.zip	Browse
Include engine files	
Include companion files	
ОК	Cancel

- o Generate all grid types from the Model Domain context menu of conceptual models
- Define particles around screens of non-vertical wells in the 3D plane perpendicular to the well stem

Defects Addressed

- Changing numeric values in color ramp settings has no effect
- Improper validation when importing a model that uses the BCF package having inactive cells with 0 thickness causes model runs to fail.
- Pilot Point values not correctly assigned using property values from the model leading to issues with preferred-value Tikhonov regularization
- PEST implementation incorrectly assumed pilot points were present in all layers and was corrected to only assign pilot points to cells/layers in their respective zone.
- ZoneBudget fails to run if Conceptual Model name has leading or trailing spaces
- Flow model translation fails if the SFR workflow schedule/data is empty. Flex will now skip SFR translation in this case.
- Project files grow after each save
- SFR2 Feature layer order and symbology does not persist after closing and reopening the project
- WEL package disables MNW2 translation in some cases
- Error assigning MNW wells to numerical model in certain cases
- · Flex fails to create child grids in one-layer grids

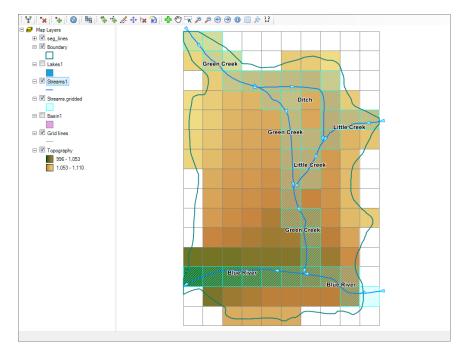
- PEST workflow does not create Variograms when some layers do not contain a zone.
- Quality and aspect ratio of exported images from 2D views was incorrect
- DRT package not included in run using Advanced translation settings
- Layer View is corrupted in some cases when viewing T=1 in View Maps step
- Surface Water Workflows are not included in cloned runs present in the original run
- Insufficient validation at translation may lead to LGR models that fail because dry cells propagate to the interface between parent and child grids.
- MODFLOW-SURFACT BCF package translation formatting is incorrect for layers with negative elevations
- Transport run window only reports up to 9999 time steps. The max number of reported time steps for a transport run is now 100,000,000.
- Cannot extract a subgrid if the project has been run previously, but not in the current session
- Importing well objects having measured depths resulting in negative elevations fails
- During transport engine translation, .BTN file does not always honor the 'Simulation time length' value entered in MT3DMS translation settings
- When a single 2D sub view is active at the view maps step, the view toolbar buttons may be hidden
- Grid color cannot be changed in Flex 2D subviews
- Export null values in dry cells/inactive cells does not respect user selection
- Error while trying to import UCN files with unknown units
- Error opening constant concentration in standalone viewers
- Error trying to access color settings in certain numerical workflows
- SFR dataset2 is missing cells during translation of model with certain topological configurations
- Property zone data entry section of Define Property Zone value is missing or clipped when high-resolution font-scaling/screen settings are used
- Compare heads functionality did not allow comparison of 3D gridded data with transient schedules
- Problems reading time units for .HDS and other 3D gridded data files from certain engines

For full version history, see the Visual MODFLOW Flex readme file at: https://www.waterloohydrogeologic.com/visual-modflow-flex-readme/

1.3.2 Version 7.0

Surface Water Workflow and Streamflow-Routing (SFR2) package support

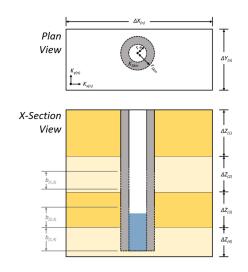
• Support for the Streamflow-Routing (SFR2) Package in Finite Difference models:

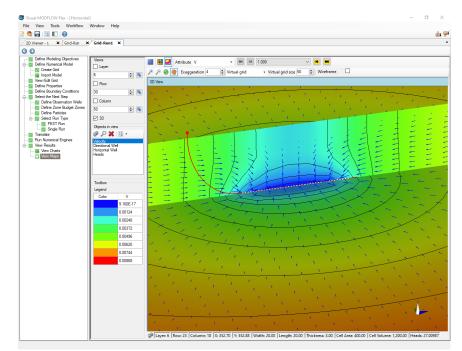


- New Surface Water workflow to develop and define connected networks of stream segments, diversions, and lakes
- o GIS editing capabilities for digitizing the surface water network
- o Surface water network attribute editing dialog for streams and lakes
- Translated SFR2 package including lake connections and 1-D vertical unsaturated flow beneath perched streams

Multi-Node (MNW1/2/I) Wells and Non-Vertical Wells

- Support for multi-node well (MNW1/2/I) packages in Finite Difference Models:
 Dynamically switch between supported well models (WEL/MWN1/MNW2)
 - Import and edit well information including head loss, well skin, and pump constraint parameter supported in MNW1/2 packages



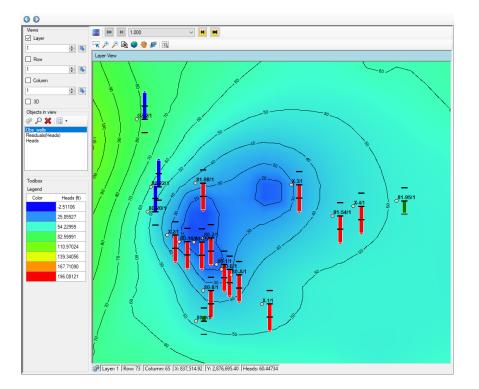


• Support for non-vertical wells (also known as deviated or horizontal) wells

- Define conceptual Wells by drawing or by assigning wellhead points
- Multi-select editing of well parameters and schedules

Calibration

- Import and/or set target residuals for head/concentration observations
- Display spatial distribution of residuals by layer or observation group at the View Maps workflow step

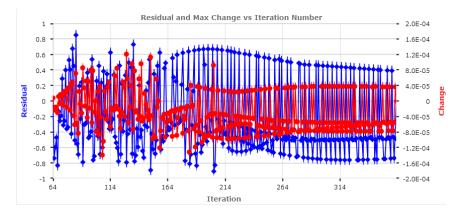


 The number of observations is included as a statistic below Calculated versus Observed calibration charts

Number of Data Points: 160 Min.Residual: -0.00022 (m) at obore_4 Time=91.3 Max.Residual: -0.23 (m) at obore_1 Time=7.738 Residual Mean: -0.022 (m) Abs.Residual Mean: 0.064 (m) Standard Error of the Estimate: 0.0063 (m) Root Mean Squared: 0.082 (m) Normalized RMS: 1.24 (%) Correlation Coefficient: 1

Model Runs

 Flow and Transport model run results are graphically displayed in real time including the global residual error and the max head/concentration change, as supplied by the active solver package settings.



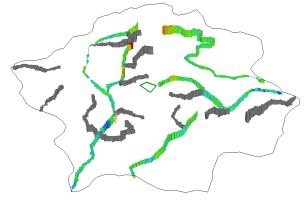
 Modified MODFLOW-USG to report solver progress in real time to the display console including global residual error

Model Import

- When importing a MODFLOW model, you can now define an offset and rotation angle for the grid to set the model in world coordinates.
- Import MODFLOW-NWT model and supported packages
- When importing files MODFLOW files, invalid values that will cause issues during a simulation (such as negative conductivities) are replaced with project default values.

•Usability and Other Enhancements

• Visualize Flow Budgets/Fluxes for MODFLOW-USG simulations



- When visualizing multi-attribute model properties such as conductivity (Kx, Ky, Kz), and Velocity (Vx, Vy, Vz, etc.) you can select the active attribute to be shown in the view and in the status bar
- Edit individual top/bottom elevations of individual cells via script when editing grid layers
- Graphically select refinement rows/columns using the mouse when editing the grid in plan view
- A link to the model files is available at the Parameter Estimation step in PEST workflow
- Translation Log is Copyable to the Windows Clipboard
- NWT translation settings include option for the IPHDRY setting
- Modified MODFLOW-USG to report solver progress in real time to the display console including global residual error

Defects Addressed

- Error during Visual MODFLOW Classic project import in projects with zero thickness cells when loading conductivity values
- The selected background color was not included in exported images of 2D views
- Property Zones listed in alphabetical order rather numerical order in the Edit Properties window

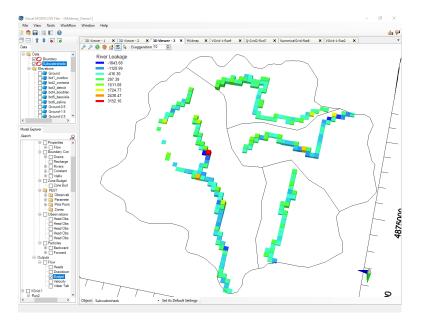
- Style settings of polygon were not retained between sessions
- Error "MS Office is not installed..." shows up during import occurs when certain versions of Office are installed
- The internal handling of time units was refactored to handle schedules and values with varying time units and scales with improved precision, accuracy, and consistency to within one second regardless of schedule duration and time units selected.
- Unable to enter negative model coordinates when defining a grid
- In some cases, when reloading a project, the "Failed to move to target step" error appears
- Voronoi grid not generated correctly when input features nearly coincide with the model boundary
- Some dialog and workflow step buttons were missing/cutoff when using lower resolution display settings.
- Unable to edit/assign boundary conditions if the duration of the schedule too large
- Background color was not saved between sessions in some views
- The option to use shapefile attribute data to define conceptual property zones not functional
- In some cases, errors prevented the export of calibration data
- Unable to convert a conceptual model to USG when certain shapefiles are used to define the model domain
- The option to use shapefile attribute data to define conceptual property zones not functional
- Errors preventing MODPATH runs in 32-Bit Versions of Flex
- Extract Subgrid failed if any model run under the original grid was previously deleted
- In some cases, concentration observations were not correctly displayed at the View Charts step
- Edit grid script failed when using shift model origin commands on variably refined grids
- Head and concentration observations were not displayed due to translation errors in some SEAWAT models
- Concentrations were not available in the Project Color Palette
- In rare cases, the pumping schedule was not correctly translated in the WEL package
- In some cases, the project could enter a state where it could no longer be saved due to the presence of larger shapefiles
- In some cases, the RT3D simulation time was not correctly translated into the BTN package
- Rerunning a model reset/removed the outputs selected in the cell inspector
- Immobile concentrations were not correctly read on successful dual domain runs of MT3DMS or SEAWAT
- PEST workflows did not correctly support overlapping zones in multi-layer models
- In some cases, observations could not be read with a Wall BC was present in the simulation
- In some cases, importing a 3D-gridded data object deleted certain property values in related numerical model(s)
- Pilot Point values not correctly assigned in distributed models, particularly in Tikhonov Regularization
- In some cases, very thin model cells in a Q-grid cause errors when converting conceptual model to a MODFLOW-USG workflow

For full version history, see the Visual MODFLOW Flex readme file at: https://www.waterloohydrogeologic.com/visual-modflow-flex-readme/

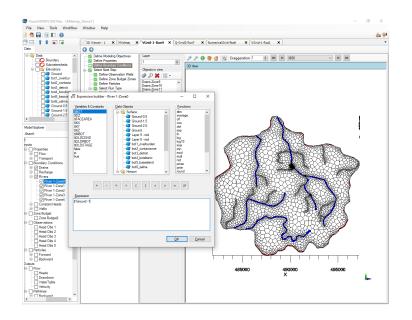
1.3.3 Version 6.1

Usability and Other Enhancements

• Boundary Condition in/outflows from the Budget file are available in 2D/3D views and the cell inspector via the Output / Budget node in the model Explorer



• You can Assign/Edit Mode Properties and Boundary Conditions using an input surface, horizon, or water table object in Expression Builder



• Expression Builder includes round and significant digit functions

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- You can zoom to an object in the Model Explorer in a 2D viewer using the context menu
- The SAMG solver is available with MODFLOW-USG
- You can specify ground surface or heads from a previous model run instead of instead of using the initial head property values at the translation step for MODFLOW-USG runs
- Visual MODFLOW Flex warns you and allows you to back up a project before irreversibly upgrading projects created in previous versions

Defects Addressed

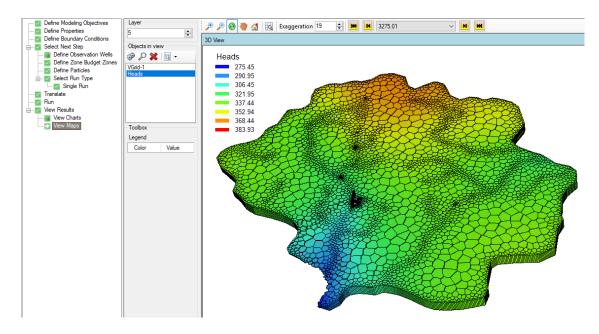
- Adding a data object such as a bitmap that is non-transparent during the grid creation process will overlay it on top of the grid rendering it invisible.
- Row/Column views for rotated grids are projected on NS/EW planes rather than on rotated model co-ordinate axes
- In some cases, surfaces generated using the model domain polygon did not fully span the model domain due to differences in numerical precision.
- LST file takes a long time to print for transient models
- Unhandled Exception when viewing certain .DXF files with unsupported components in a 2D Viewer
- Performance Issues on Project Load and Reload
- In some cases, not all observations are included when exporting data from the Calc. vs Obs. Chart
- In some cases, linear boundary condition features were skipped during conceptual to numerical model conversion.
- Concentration output nodes are not always created in RT3D runs
- Conceptual BCs assigned to the model sides not assigned as expected following conceptual to numerical model conversion to a finite difference grid if the grid cells are thin and/or there are steep gradients at the model edge.
- Uncaught exception visualizing Fluxes when budget file is removed
- View Maps not showing heads output
- Can't assign wells using Wells data object on Q-Grid
- Well Edit form dives under the main Flex window
- Only the first stress period values for bed leakance were included in LAK package translation

For the full version history, see the Visual MODFLOW Flex readme file at: https://www.waterloohydrogeologic.com/visual-modflow-flex-readme/

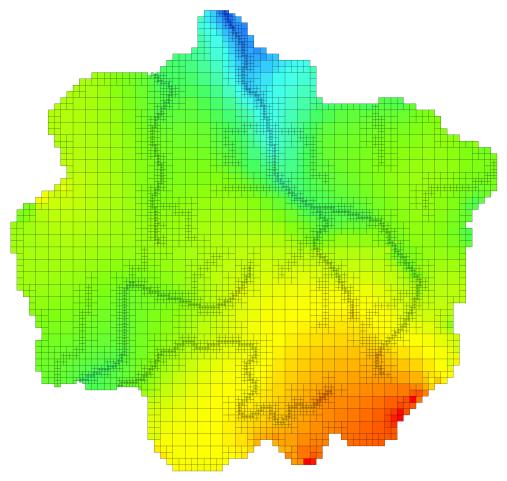
1.3.4 Version 6.0

Working with Unstructured Grid Models

- Build your unstructured MODFLOW-USG model using the same workflow steps and tools as in a structured Finite Difference model:
 - Define Modeling Objectives
 - Define Model Properties
 - o Add Boundary Conditions
 - Define ZoneBudget Zones
 - o Define Particles



• Define Quadtree Grids (Q-Grids)

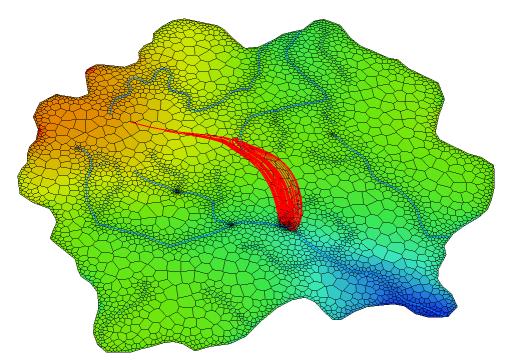


• Refine vertical layers when creating unstructured grids

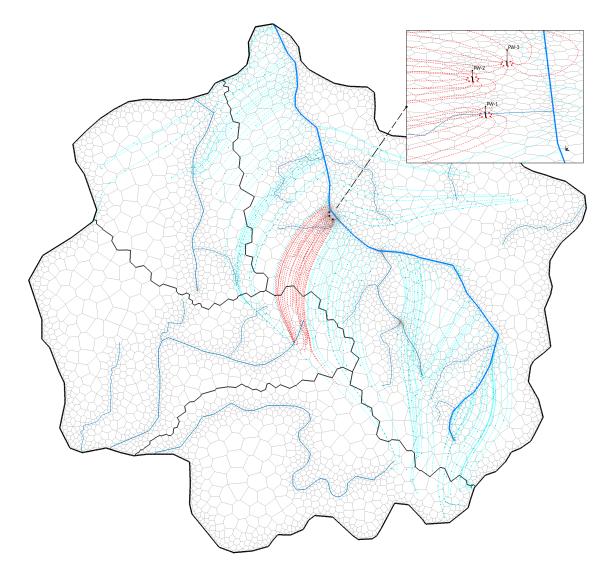
- Make use of advanced translation settings which provide greater flexibility in how your model simulations are formulated
- Support for the Ghost Node Correction (GNC) package
- Flex is now installed with MODFLOW-USG v1.4, the latest official USGS version as of the release date of Flex 6.0.

Particle Tracking

• Support for mod-PATH3DU^{*}, which enables particle tracking in unstructured grid (MODFLOW-USG) models:



- Enhanced particle tracking capabilities for MODPATH and mod-PATH3DU allowing you to define:
 - o Groups of particles that can be tracked and visualized separately
 - o Separate particle release times for each particle group
 - \circ Locations of particles based on existing or drawn point, polyline, polygon, or well features

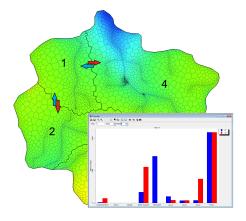


- o Particles in the cross-section (row/column) views of Finite Difference grids
- o Particle elevations based on layer(s), surface(s), or a specified constant elevation

* **Note**: mod-PATH3DU is a free utility developed by S.S. Papadopulos, Inc. (SSPA) that must be downloaded and installed separately from the SSPA website. Version 2.1 and higher are supported. Note, that Version 3.0 includes improvements to handle a wider variety of unstructured grids

ZoneBudget

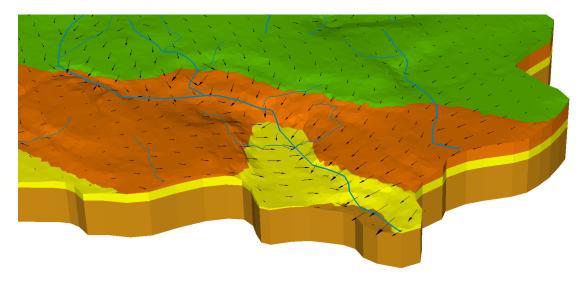
• ZoneBudget is now supported in unstructured MODFLOW-USG models



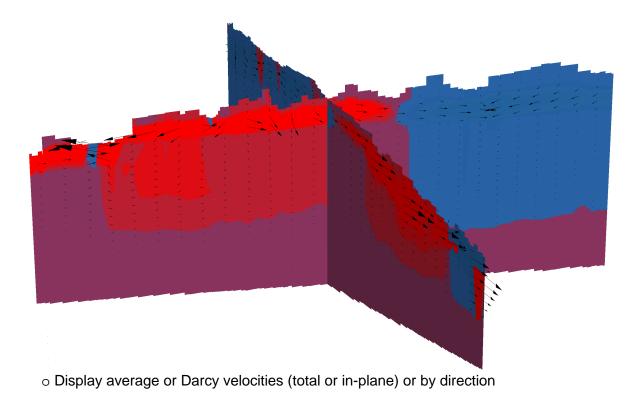
• You can use point, polyline, or polygon features to define Zone Budget zones and Zone IDs can be specified using feature attributes

Visualization and Settings

Visualize velocity vectors in finite difference and unstructured grids. View:
 o In-plane velocity vectors



o Color maps of out-of-plane velocities



- Specify a line feature along which to show cross-sectional color maps of unstructured grid model properties and outputs
- Cell Inspector now includes Layer/Model Top and Bottom elevations, and the magnitude and X-, Y-, and Z-components of the average/Darcy groundwater velocity
- When creating horizons, you can preview how the rules will be enforced in the 3D Viewer rather than viewing the raw surfaces.

Packages, Properties, and Boundary Conditions

- Field calculator/expression builder for editing model properties and boundary condition includes:
 - cell geometry variables: Cell Bottom (\$BOT), Model Bottom (\$MBOT), Cell Thickness (\$DZ), Cell Width (\$DX), and Cell Length(\$DY) and
 - o additional math functions: LOG, LOG10, NOT, ABS, DOT
- Copy Model (Flow/Transport) Properties and Boundary Conditions to from one Layer, Row, or Column to other Layers. Rows, or Columns
- Edit cells (active/inactive, zone budget) in row/column views.

Data Import/Export

- You can import distributed property values from Classic Models
- Map elevation to a field in source data when importing points from shapefile
- Model outputs including groundwater heads, drawdown, velocity, and concentrations can be exported to text files
- Export contours as polyline shapefiles

Usability and Other Enhancements

- Head and Concentration Observations can be specified as separate groups so that you can view and filter these separately at the View Charts step
- Performance improvements on project open and close operations for larger projects.
- Output Control file translation supports the use of keywords or codes and the standard or compact budget formats to provide support for both MODPATH and RT3D.
- Added MT3D-MS and RT3D summary output (.OT) files to the open files dialog at the model run step

Defects Addressed

- Intermittent and unhelpful translation error "Vmac is running in the task bar, please close it and try again".
- Deleting particles by drawing a box does not actually delete particles
- Well schedule not translated correctly if the project time unit is not in days
- In some cases, particularly if the whole output water table exceeds the model ground surface it was rendered at Elevation=1
- Modifications to a pumping well boundary condition propagate to all runs under the same grid
- Concentration observations contained incorrect column names
- Project Clean-up/Remove orphan objects from model
- If all boundary conditions of a given type were deleted, they would still run in the model due to advanced run settings. You are now prompted to remove the translated file or back-it up so that it no longer runs in the model
- In some cases, the schedule for pumping wells with relative times does not import correctly
- In some cases, assigning a schedule to a conceptual boundary condition results in an error message that the schedule occurs before the model start date even if this is not true
- Concentration observations incorrectly handled for simulations with multiple species
- Transient Fluxes (Model Results) are not shown or exported, only Flux from first time step.
- Fluxes not displaying properly in 3D Viewer
- Cells remain active if boundary condition is applied to 'Top' of model domain
- MODFLOW-USG, BCF package fails to translate if property values are edited
- When using a uniform grid, the CM->NM conversion does not add conceptual BCs assigned to model top to Layer 1 rather than the upper-most active layer
- When importing heads file as 3D gridded data to a Rotated Grid Project, error "Object reference not set to instance of object appears"
- Inconsistent/compound units are not correctly converted for certain RT3D reaction parameters
- Water table for USG does not take ponding into account
- Reinstalling Visual MODFLOW Flex does not replace MODFLOW-SURFACT with the demo version in the engines folder

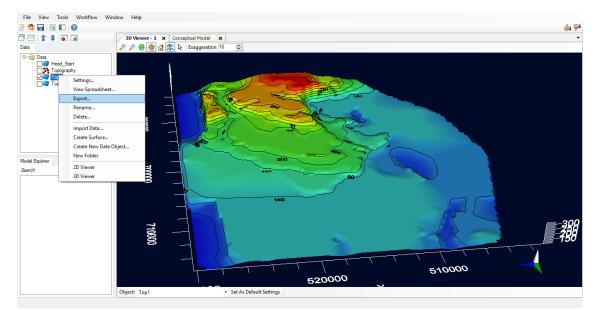
- Flex does not always cleanly delete elements from the Model Explorer, resulting in large file sizes
- In some cases, MODFLOW-USG conceptual model conversion results in incorrect parameter values, and causes parameter editing to fail
- Out of memory error when attempting to display certain DXF files in 2D view of Flex viewer or standalone 2D viewer
- Multiple Lake BCs result in a multiple key error upon translation

For full version history, see the Visual MODFLOW Flex readme file at: https://www.waterloohydrogeologic.com/visual-modflow-flex-readme/

1.3.5 Version 5.1

Data Import/Export

• Surfaces created in Visual MODFLOW Flex can be exported as Surfer ASCII grid files (.GRD) for use in other Visual MODFLOW Flex projects and other software packages (e.g. Surfer, ArcMap, QGIS).

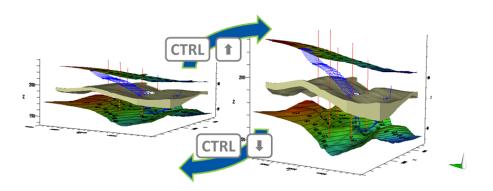


• Pumping Wells in Visual MODFLOW Flex numerical models can be imported as text files (.CSV) using the same format that they are exported from Flex projects allowing you to transfer Wells between projects.

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Visualization and Settings

Vertical exaggeration in 3D views can be manipulated by keyboard commands:

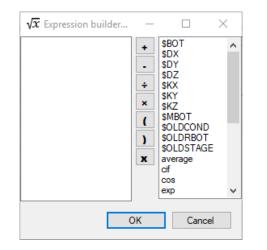


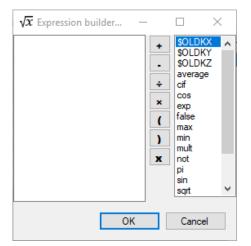
The following keyboard commands adjust the vertical exaggeration in 3D-Views:

- <Ctrl><Up> increase vertical exaggeration by 1
- <Ctrl><Shift><Down> decrease vertical exaggeration by 10
- <Ctrl><Up> increase vertical exaggeration by 1
- <Ctrl><Shift><Down> decrease vertical exaggeration by 10
- <Ctrl><Home> set to vertical exaggeration to 0

Packages, Properties, and Boundary Conditions

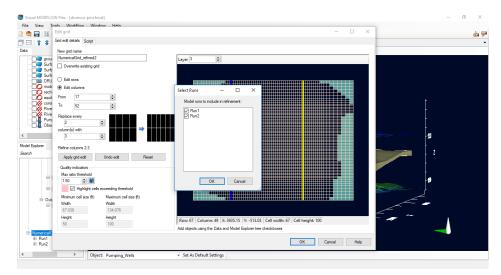
• Field values for Properties and Boundary Conditions are available as variables in the Expression Builder





Grid Editing

• You can now specify which numerical model run(s) are carried over when performing grid edits.



Defects Addressed

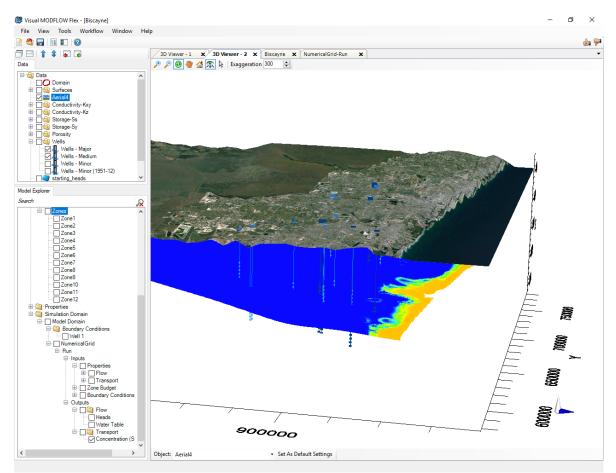
- In some scenarios (for instance if CHD cells are specified at the very bottom of the model [such as in the Henry model]), the parallel version of SEAWAT may have convergence problems that cannot be resolved by changing solver parameters.
- SEAWAT engine run output was truncated and formatted incorrectly.
- Concentration values of -1 in the specified concentration boundary condition (indicating the species should be skipped) were incorrectly translated to the SSM file as 0.
- Error in translating diffusion arrays to the DSP package when specifying the Multidiffusion option in MT3D-MS or SEAWAT runs.
- In rare occasions, property zones were set to -1 and uneditable.
- In some cases, successive model translation times increased due to a memory leak.
- In ZoneBudget runs, Flex does not read in values for zones that are not directly adjacent to Zone 1.
- Errors thrown if user skips straight to Translate without selecting an engine.
- In some cases, changes to stress periods do not update instantly to the translation settings resulting in incorrect translated time discretization and/or output control (.OC) files, following changes.
- In some cases, PEST results will not update correctly into a new run.
- An error is shown when user clicks [...] button to change the path to Previous MODFLOW Run HDS file if the HDS file is not present.
- Hitting Apply in the Settings dialog for a concentration doesn't update the BC view properly.

For full version history, see the Visual MODFLOW Flex readme file at: https://www.waterloohydrogeologic.com/visual-modflow-flex-readme/

1.3.6 Version 5.0

-SEAWAT

Visual MODFLOW Flex now supports <u>SEAWAT</u> (v4.00.04), a three-dimensional variable density flow and multi-species solute transport model developed by the USGS, based on a combination of MODFLOW and MT3D-MS. Version 4 of SEAWAT also supports viscosity effects and heat transport.



Source data courtesy of the USGS (SIR2016-5022)

The following SEAWAT flow packages are supported in Visual MODFLOW Flex:

- BAS6 Basic Package
- DIS Discretization Package
- BCF6 Block-Centered Flow Package
- LPF Layer Property Flow Package
- **RCH** Recharge Package
- EVT Evapotranspiration Package
- WEL Well Package
- DRN Drain Package RIV River Package
- GHB General-Head Boundary Package
- FHB Flow and Head Boundary Package
- CHD Time-Variant Constant Head Package
- LAK Lake Package (LAK3)
- HFB6 Horizontal Flow Barrier package (HFB6)
- **OBS** Observation
- HOB Hydraulic-Head Observation
- GMG Geometric Multi-Grid Solver
- PCG Pre-conditioned Conjugate Gradient Solver (PCG2)
- WHS BiCGSTAB-P Matrix Solver

 LMG - Link Multi-Grid package for using the SAMG (Systems Algebraic Multi-Grid) Solver

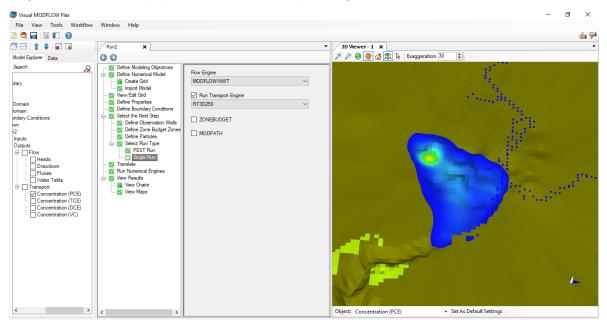
The following SEAWAT transport packages are supported in Visual MODFLOW Flex:

- VDF Variable Density Package
- VSC Viscosity Package
- **BTN** Basic Transport
- ADV Advection
- DSP Dispersion
- SSM Source/Sink Mixing
- **RCT** Reaction Package
- GCG Generalized Conjugate Gradient Solver

NOTE: Advanced Translate/Run Settings (see below) enable partial support for simulating additional processes/packages (e.g. subsidence, drain return) developed outside of Flex.

•RT3D

Visual MODFLOW Flex now supports <u>RT3D</u> (v2.50), an advanced reactive transport engine based on the popular MT3DMS transport engine.



The following RT3D reaction modules are supported in Visual MODFLOW Flex:

- Instantaneous aerobic degradation of BTEX.
- Six Species, First-Order, Rate-Limited, BTEX Degradation using Sequential Electron Acceptors
- Rate-Limited Sorption
- Double Monod Model
- Sequential First-Order Decay (up to 4 species, e.g., PCE/TCE/DCE/VC)

Aerobic/Anaerobic PCE/TCE Dechlorination

Visualization and Settings

• **Cell Inspector**: View and inspect structured and unstructured models at the cell-level using the new cell inspector, available in the workflow viewers. The cell inspector displays cell values for user-specified input and output data fields.

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- Positio					
🖃 SE	AWAT				
	Layer	15			
: :	Row	1			
	Column	200			
	ModelX	1995	m		
	ModelY	100	m		
	ModelZ	-145	m		
	WorldX	1995	m		
	WorldY	100	m		
	WorldZ	-145	m		
Bound	ary Conditions				
🖻 Co	nstant Head 1				
	Starting Head	0	m		
	Ending Head	0	m		
	Density	1000	kg/m^3	3	
	Salt	35000	mg/L		
	Temperature	5	mg/L		

• Status Bar: Cell dimensions have been added to the status bar.

Layer: 12 Row: 384 Column: 15 X: 800636.32 Y: 591064.42 Width: 500 Length: 500 Thickness: 53.5570036997129

• Time-Picker: A time-picker is now available for unstructured grid workflow viewers.

-	N	90	~	M	H
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• Layer-Picker: A layer-picker is now available for unstructured grid workflow viewers.

Layer	
1	-

-Workflows

• Additional Translation/Run Settings: Added advanced settings for all supported engines (excluding MODFLOW-USG) so that you can specify whether individual

packages are translated and/or run with the model, which provides the flexibility to integrate your own package input files within the Flex environment.

Settings	Translation Log	DIS	LPF	BAS	OC	WEL	VDF	VSC	CHD	BT3	AD3	DP3	RC3	GCG	SS3	IN	
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	LPF																
	LVDA			C11 - 3													
	MNW1			CUnit CUnit													
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Property and Boundary Condition Tools

• **Field Calculator**: Populate boundary condition fields using a calculator that includes an expression builder dialog to facilitate the inclusion of variables based on your model's properties (e.g. grid dimensions, elevations).

\sqrt{x} Expression builder - River 1		_		\times
sqrt(\$KX*\$KY)	+ - + () X ^y	SBOT SDX SDY SDZ SFACEARE SFACEARE SFACEARE SFACEARE SKY SKY SKZ SMBOT SS SUCTOCON average cif cos exp false	A_TOP A_WEST	<
		ОК	Cancel	

• **Dispersion Parameters**: Values can be edited in the Dispersion Parameter Dialog using copy, paste, and fill commands.

۲	Dispersion Paramete	rs		- 0	×
	🔲 🖨 📋				
	Layer	Horiz/Long Dispersivity	Verti/Long Dispersivity	Diffusion Coeff. (m^2 / day)	^
•	1	0.1	0.1	1E-10	
	2	0.1	0.1	1E-10	
	3	0.1	0.1	1E-10	
	4	0.1	0.1	1E-10	
	5	0.1	0.1	1E-10	
	6	0.1	0.1	1E-10	
	7	0.1	0.1	1E-10	
	8	0.1	0.1	1E-10	
	9	0.1	0.1	1E-10	
	10	0.1	0.1	1E-10	
	11	0.1	0.1	1E-10	_
				OK Cance	

Usability and Other Enhancements

- Easy Classic Importing: Import your Classic project into Visual MODFLOW Flex directly from the file menu.
- Import Classic Concentrations: Boundary condition concentrations are now imported from Classic Projects.
- Animate Relative times in 3D views: in 3D View animations, the time stamp label for heads can be specified in relative or absolute time.
- **Descriptive Title Bars for Settings Windows**: settings windows now display descriptive window titles including the data layer and viewer the settings to which they apply.
- **Rename Objects**: objects in the Data Explorer and most objects in the Model Explorer can be renamed.
- Feedback Button: added anonymous feedback buttons so that you can easily report what features you like or don't like.
- **SAMG Solver**: added a single-processor version of the SAMG solver for Visual MODFLOW PRO users.

Defects Addressed

 Defining BCs along irregular polylines that are close to the active model limits produced unexpected results

- Reorder Tool was missing in some views
- The Show/Hide Gridlines button and associated toolbar disappeared intermittently from the viewer
- Well Data import failed without warning the user that the pumping schedule had inconsistencies, including pumping start date before model start date or pumping start date after pumping end date
- User could not assign polygon attribute data to conceptual recharge/evapotranspiration elements
- Problem(s) with Time Series Viewer
- Multiple PEST Workflows could be created for the same model run which corrupted the PEST workflow.
- · Multiple issues in the advanced run/translation settings
- PCG Solver translation settings of the PCG2, PCG4, and PCG5 solver packages for MODFLOW-SURFACT models

For full version history, see the Visual MODFLOW Flex readme file at: https://www.waterloohydrogeologic.com/visual-modflow-flex-readme/

1.3.7 Version 4.1

Visualization and Settings

- 2D/3D View Keyboard Navigation: Navigate in the active 2D or 3D view using the keyboard. Arrow keys pan the view, +/- keys (on the number pad) and page up/page down keys zoom in and out. In an active 3D view, the <shift>+arrow up/down keys changes the inclination of the model relative to the horizon and <shift>+arrow right/left rotates the model about the vertical axis.
- **Custom Contours**: Customize contours in 2D, 3D, and Flex Viewers by setting start and finish contour values for contour lines and isolines. You can also specify a contour interval. Changes in one part of the Flex Viewer are reflected in the other parts.
- **3D View Setting Defaults**: Create and Save Project-Specific Default View Settings for each each data type in the 3D Viewer.
- **Time-Series Viewer**: View time series data such as heads, saturation, and concentration at points within transient models without specified observation points.

Workflows

• **Modeling Objectives**: Modeling Objectives for Transport Simulations can be changed at any time, not just during initial setup or conversion.

 Model Settings for Translate/Run: You can now specify whether individual packages are translated and/or run with the model, which provides the flexibility to use your own packages similar to the advance settings in Classic for model translate/run.

Grid Editing Enhancements

• Cell Size Control for Conceptual Models: Similar to numerical grids, you now have full control over the grid cell size specification during initial grid creation; you can set grid cells to whole numbers for ease of calculation and reporting.

Property and Boundary Conditions

- Boundary Conditions in LGR Models: Boundary conditions that span the parent/child grid interface(s) in an LGR model can be specified in both the Conceptual and Numerical workflows.
- **Dual Domain mass transfer**: Flex now supports dual domain mass transport modeling through the MT3DMS and MODFLOW SURFACT (see below) transport engines.
- Unsaturated Zone Flow (UZF) Package: Flex now supports 1-D unsaturated flow associated with the UZF package.

Updated Engines

- Upgraded MODFLOW 2005: Flex is now packaged with MODFLOW-2005 v1.12.00, the latest official USGS version as of the release date of Flex 4.1.
- Upgraded MODFLOW NWT: Flex is now packaged with MODFLOW-NWT v1.1.2, the latest official USGS version as of the release date of Flex 4.1

MODFLOW SURFACT

 Added Support for MODFLOW SURFACT: Visual MODFLOW Flex now supports MODFLOW SURFACT Version 4.0, a fully-coupled flow and transport engine developed by Hydrogeologic, Inc. which features many robust methods and enhanced simulation capabilities for handling complex saturated/unsaturated subsurface flow and transport processes. Based on the USGS modular groundwater flow model, MODFLOW, it supports the following packages:

Package	Pack	Description	Ext.
Туре	age		
	BAS4	Basic Package	BAS
Flow and	BCF4	Block-Centered Flow Package	BCF
Transport	BTN1	Basic Transport Package	BTN
Processes	TMP1	Time-Varying Material Properties Package	TMP
	CHD	Time-Variant Specified Head	CHD
	DRN	Drain Package	DRN
	EVT	Evapotranspiration Package	EVT
	FHB	Flow and Head (Time-Varying) Boundary	FHB
	FWL5	Multi-Node Fracture Well	FWL
Flow and	GHB	General-Head Boundary	GHB
Flow and Transport Boundary Conditions	HCN1 Prescribed-Head- Concentration Boundary		HCN
	HFB	Horizontal Flow Barrier (Wall)	HFB
	LK3	LAK	
	PCN1	Prescribed-Head- Concentration Boundary	PCN
	RSF4	Recharge-Seepage Face Package	RCH
	RIV	River Package	RIV
	WEL	Well Package	WEL
Observations	HOB	Head Observation Package	HOB
Observations	OBS	Observation Nodes	OBS
Output Control	OC	Output Control	OC
	PCG5	Preconditioned Conjugate Gradient Solver	PCG
	SIP	Strongly Implicit Procedure	SIP
Solvers	SAM G	Algebraic Multi-Grid Solver	LMG
	GMG	Geometric Multi-Grid Solver	GMG
	WHS	BiCGSTAB-P Matrix Solver	WHS

NOTE: MODFLOW SURFACT was developed by Hydrogeologic, Inc. and is sold as a separate add-on for Visual MODFLOW Flex. A demo-version that supports model grids of up to 10,000 cells is included for evaluation purposes. Additional packages are supported by SURFACT and may be developed outside Flex.

Usability and Other Enhancements

- Undock/redock Tabs: Tabs can be undocked as separate windows. Simply drag and drop or right-click on the Tab name and select the "Undock Tab" option and you can place the new window anywhere on your monitor screen(s). Redock a window back to the main program window using drag and drop or right-click and select "Dock Tab" option.
- Explorer Support: Open a Visual MODFLOW Flex .AMD file directly from Windows Explorer.
- .Net Framework 4.6.1: now bundled with Flex installation

- About/Splash Screen: Version and Build number are displayed on the Splash Screen and on the About Screen.
- Improved Performance: Improved memory handling and performance enhancements

Defects Addressed

- Could not edit or define a Boundary Condition when multiple grids were present as part of the same LGR grid
- Inconsistency between calculating and displaying leakance in the lake boundary condition when using certain time units
- Some PEST runs were not successful due to incorrect observation files.
- Issue when importing time schedules for recharge package
- Translation issue when importing some Visual MODFLOW 2010.1 Classic projects into Flex.
- Progress bar does not provide adequate feedback when opening large projects
- Issue with extracting multiple species from sub-grids for MT3DMS runs
- Toolbox was blank after translating/running the model and clicking Define Properties step
- Translation issue in MT3DMS RC3 file for bulk density values when using inconsistent units
- Improved feedback/reporting for certain engine runs that do not converge

For full version history, see the Visual MODFLOW Flex readme file at: https://www.waterloohvdrogeologic.com/visual-modflow-flex-readme/

1.4 How to buy

You can buy Visual MODFLOW Flex directly through your local sales representative (via email/phone), from one of our global distributors, or online through the shopping cart on our website using a credit card:

Waterloo Hydrogeologic Sales Team:



sales@waterloohvdrogeologic.com



+1-519-746-1798

Global Distributors:

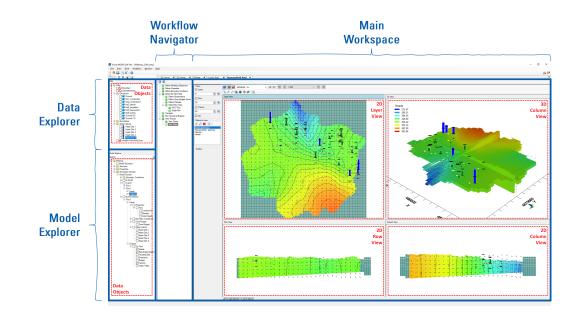
www.waterloohydrogeologic.com/global-distributors/

Online Store:

2 Program Overview

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In order to become the most efficient and effective in the Visual MODFLOW Flex environment, it is recommended that you familiarize yourself with a few simple concepts, terminology, and where you can find and access things.



Data Objects

All of the data that you interact with in Visual MODFLOW Flex are referred to as data objects. These can consist of:

- Raw Data that you have:
 - Imported: From polyline or polygon shapefiles, wells from a spreadsheet, surfaces from Surfer .GRD, etc.
 - Created: Through digitizing points, polygon, or polylines or by interpolating points to create surfaces
- **Conceptual Data Objects**: These are generated as you progress through the conceptual modeling workflow, and include:
 - Horizons, Structural Zones, Property Zones, and Boundary Conditions.
- Numerical Model Data Objects: These are generated as you progress through a numerical modeling workflow, and include:
 - Input: Numerical Grid, Properties (Conductivity, Initial Heads, etc..), Boundary Conditions (a group of river cells, drain cells, pumping well cells, etc..), Observation Wells, Zone Budget zones, and Particles.
 - Output: Calculated Heads, Drawdown, Pathlines, etc.

Each data object will have a check box beside it, allowing it to be displayed in different 2D/3D viewers. Data objects can be re-ordered, renamed, or grouped into data folders. To create a data folder, right-click in the Data are Object explorer and select New Folder. Data folders can be renamed.

Each data object also has Settings which can be accessed by right-clicking on the data object in the tree, and selecting Settings. The settings provide access to general properties (statistics, file origin, etc.) and Style settings (symbol colors, shape, labeling, etc.) for those objects displayed in an active viewer. For more details, see <u>Data Settings</u>.

Many wizards and dialog boxes in Visual MODFLOW Flex require you to select data objects from the Data Explorer or Conceptual Model Explorer, e.g., when defining horizons, creating property zones, and assigning attributes to boundary conditions.

When you see a Blue Arrow located next to an input field in a dialog box or a wizard, this means that a data object selection is required. Simply click the appropriate data object from the Data Explorer or Conceptual Model Explorer and then click the Blue Arrow button to insert the data object into the input field.

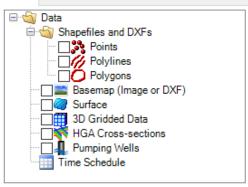
Data Explorer

The Data Explorer contains all of the imported and created data objects that can be used to build your conceptual and numerical model.

The Data Explorer supports the following types of Data objects:

- Points
- Ø Polylines
- O Polygons
- Site Maps (Georeferenced Images or DXF files)
- Interpretation
 Interpretation</l
- I 3D Gridded Data
- Mathematical Hydro GeoAnalyst (HGA) Cross-Sections
- 4 Wells
- 🛄 Time Schedules

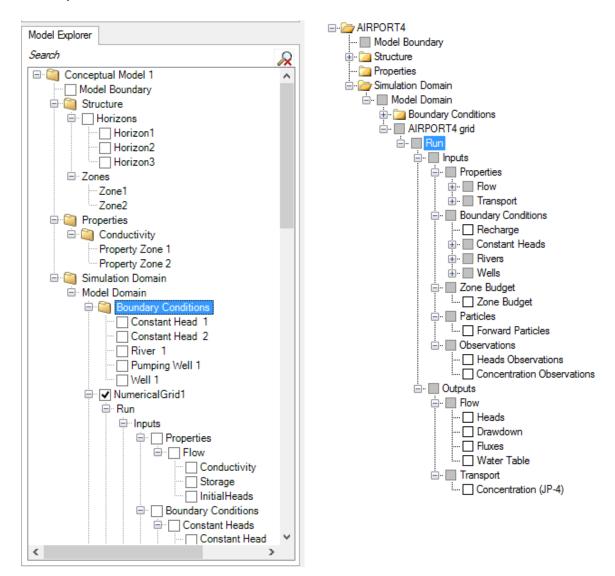
For more details, see Working with Your Data.



Model Explorer

The Model Explorer contains all of the <u>Conceptual Models</u> and numerical models (either <u>Finite Difference</u> or <u>Unstructured</u>), and corresponding data objects for your project. To help you locate items in the model explorer, we have included a search option which will automatically filter the items in the tree based on what you type.

Numerical Model Tree



Conceptual Model Tree

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= 2D/3D Viewers

Data objects can be displayed in one or more of the following viewers:

- 2D View: Plan view; ideal for GIS data, surfaces, well locations, images, etc.
- **3D View**: Ideal for data that have X,Y and Elevation (Z) values defined: such as Structural Zones, Wells, Pathlines, Heads along a cross-section, etc.
- "Flex" View: Ideal for complex views and available in the numerical modeling workflows, the Flex viewer consists of a combination of a Layer, Row, Column, and 3D sub-views. The individual sub-views can be shown/hidden.

For more details, please see <u>Visualizing Data in 2D/3D</u>

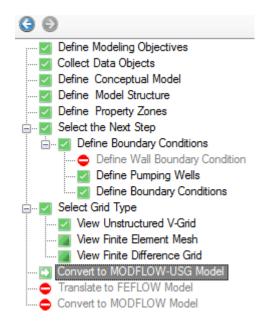
Workflows

Groundwater modeling consists of a series of steps that must be completed in a particular sequence in order to achieve a specific goal. In Visual MODFLOW Flex, these steps are presented in a workflow. In the Workflow window, you see the steps that make up a workflow and at each step there is a corresponding GUI with which you interact. The benefits to you as a modeler are unlimited:

- **Simplicity**: You know where you are and where you have to go. This dramatically reduces the learning curve.
- Accessibility: all the actions you need are available at your fingertips; no more hunting for an option deep inside a menu.
- **Convenience**: modeling is iterative and requires a frequent amount of flipping between input, run, and results. The workflow GUI simplifies these back-and-forth tasks.

In Visual MODFLOW Flex, there are separate workflows for Conceptual Modeling, Numerical Modeling (either <u>Finite Difference</u> or <u>Unstructured</u>), <u>Surface Water</u>, and for <u>PEST</u> (Parameter Estimation/Sensitivity Analysis).

The workflow panel contains a toolbar and a list of steps required for your current workflow.



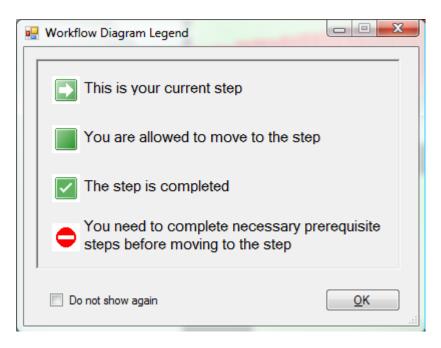
Navigating a Workflow

G Go to the Previous Step in the workflow

Go to the Next Step in the workflow

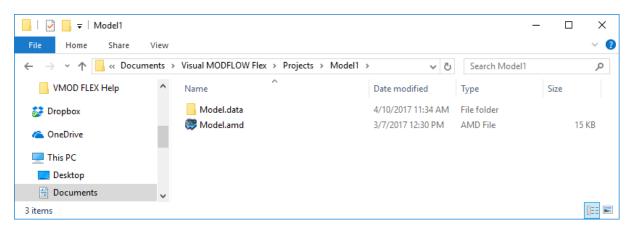
Workflow States

Beside each state in the workflow there is a corresponding icon. The icon helps you to identify which is your current step, which steps have been completed, and which steps you may proceed to next. The image below provides an explanation of this.



File Structure

Visual MODFLOW Flex projects consist of a project file and associated folders with the same base name. For example, if you have a Visual MODFLOW Flex project called "Model", the entire project consists of the file "Model.amd" and the folder (and its contents) in the same path location called "Model.data".



In order to transfer or manually backup a Visual MODFLOW project from one file location to another, you will need to copy both the .AMD file and its associated folder data to the new location. Visual MODFLOW Flex also includes a <u>backup utility</u>.

▲ CAUTION: The Visual MODFLOW Flex file structure includes many managed data files, which are continuously read from and written to the project data folder. For best performance and stability, it is strongly recommended that you only save projects to local disk folder that are NOT managed by file synching/sharing services (such as

OneDrive, SharePoint, DropBox, Box, etc.). These file synching/sharing services are not aware of the Visual MODFLOW Flex file structure and are not likely to not keep up with the files as they are created which will likely lead to project corruption. Saving projects over slow network connection may cause similar issues.

2.1 Main Menus and Toolbars

The following sections describe the various menu and toolbar options in Visual MODFLOW Flex.

-Menu Items

File Menu

The File menu provides access to standard operations such as open, save, save as, and close project. The file Menu can also be used to import data from external sources and modify project settings. You will find the last few models you have opened so you can quickly re-open them.

File Operations:

New Project <CTRL+N>: Opens the create new project setup dialog.

Open Project <CRTL+O>: Opens an existing project. Note: only one project can be open in Flex at a time.

Import Project <CTRL+I>: Imports a Visual MODFLOW Classic (*.vmf) file.

Close: Closes the active project

Project Operations:

Save Project <CTRL+S>: Saves the active project to its current location.

Save Project As <F12>: Saves the active project in a selected location.

- **Project Settings**: Opens the <u>Project Settings</u> dialog, which stores model setup and project meta-data information: including model default values, units and coordinate system.
- **Import Data <CRTL-D>**: Opens the <u>Import Data</u> dialog to add external data to your project.
- **Backup Project**: Opens the <u>Backup Project</u> dialog to create a zip archive of your current project

- **Open Project Location**: Opens a windows explorer window at the path of your current project
- **Recent Project List**: A list of the most recently saved projects will be shown. Selecting any of the projects in the list will close any active project (upon user confirmation) and open the selected project.

Exit <Alt+F4>: Exits Flex - you will be prompted to save your project if one is open.

View Menu

The View menu allows you to show/hide the Data and Model Explorer panes <F11> and the Workflow tree <F4>.

Tools Menu

The Tools menu provides the following options:

- **Free Memory**: allows you to free up some memory usage if you have been running a number of high-demand, 3D visualization operations
- **Free Storage**: allows you to free up some disk space cleaning up files in the project that are no longer used and includes an option to backup these files.
- **Preferences**: opens the <u>Preferences</u> settings dialog which allows you to adjust the settings for 3D Viewers and for Flex in general.
- **Restore System Settings**: Use this option to reset Visual MODFLOW Flex to factory style settings. This option may sometimes be useful or required to enable certain newer visualization/style settings in projects that were created in older versions of Flex.
- **Project Color Palette**: Visual MODFLOW Flex provides an option to use Project-wide Color Palettes. This is useful when you have multiple data objects that are rendering the same attribute (eg. heads from different model runs, conductivity distributions), and you want to make qualitative comparisons between these. This is challenging when each data object has its own min and max values and are colored based on this. However, it becomes much easier when these data objects all read from a common color palette.

*	Project Color P	alette	×
	Attribute HEADS	36	60.00000
	Max Value 360.00000		
	Min Value		
	280.00000	28	30.00000
		ОК	Cancel

The Project Color Palette settings allow you to set the min/max values for various attributes; these can then be used for various data objects and viewers throughout the project.

To enable the Project Color Palette option for a specific data object, this must be enabled in the Color by Attribute page; see <u>Color by Attribute</u> for more details.

Workflow Menu

Allows you to open an existing workflow in your project:

- Conceptual Modeling workflow,
- Unstructured Grid Numerical Modeling workflow,
- Finite Difference Numerical Modeling workflow,
- Surface Water workflow, or
- PEST workflow

When you select the appropriate item, the associated workflow window will load.

You can also create a new Conceptual Modeling Workflow or a new Finite Difference Numerical Model workflow; other workflow types can only be created as part of an existing conceptual or numerical modeling workflow. See individual workflow chapters for more details.

Window Menu

The Windows menu provides the following options:

New 2D Window: creates a new empty standalone 2D View window

New 3D Window: creates a new empty standalone 3D View window

- New Time Series Window: creates a new empty Time Series View window
- **New Calibration Dashboard**: creates a new calibration dashboard from the selected run(s).
- **Reset Windows to Default Location**: (re)docks all windows (workflows, views, and dashboards) as tabs in the Main Workspace
- **Open**: Allows you to manage existing views, including open, rename, and delete existing standalone 2D, 3D, and Flex views

Help Menu

Provides links to help topics, webhelp, and online resources. The Just-In-Time Help will display a small help panel below most steps in the workflow window.

- Help Topics (F1): opens the built-in help documentation including tutorials and getting started guides
- Web Help: opens the online-help documentation
- Release Notes: opens the online documentation for the changes associated with each version
- **Online Support and Resources**: opens the online page for accessing technical resources and contact information for technical support
- **Checks for Updates**: calls out to Waterloo Hydrogeologic's webpage to see if updates are available.
- **Show Error Log**: opens the Visual MODFLOW error log, which can be useful in helping technical support diagnose and pinpoint problems, if they arise.
- **Error Settings**: allows you to specify the level of detail to log (Error, Warning, Information, Verbose) and size of the error log. By default, the Flex log may grow to 25 Mb and logs at the "Warning" detail level. Once the specified capacity is reached, the error log is reset.
- **Show System Information**: opens a text file with system configuration information, which can be useful in helping technical support diagnose problems, if they arise.
- **About...** launches the About Screen, which shows the version and build you are using along with your registration details (name, company, serial number).
- **Licensing Help** will load the online help for working with licensing. For more details on licensing, please refer to the <u>Licensing Guide</u>.

Main Toolbars

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Below the main menu, there are two main toolbars:

Project Toolbar

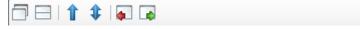
The toolbar in the first row contains application/project level options; from left to right, these options are:



- New Project
- Open Project
- Save Project
- Show/Hide the Model Explorer and Data tab
- Show/Hide the Workflow Tree
- Help: opens the built-in help documentation
- Thumbs Up/Down: opens a window that allow you to submit anonymous feedback and product feature requests

Data Panel Toolbar

The toolbar in the second row contains options for adjusting the Data tab and Model Explorer; from left to right, these options are:



- Combine Data tab and Model Explorer into one view, separated by tabs
- Separate the Data tab and Model Explorer into one frame above the other (factory default setting)
- Collapse All (levels of the tree)
- Collapse to Selected item on the Model Explorer
- Dock Model Explorer to the left side of the window
- Dock Model Explorer to the right side of the window

2.1.1 Project Settings

The project settings dialog allows you to adjust various project-specific settings in Visual MODFLOW Flex:

- Project Information Tab
- Project Coordinates
- <u>Units</u>
- Model Defaults

Project Information Tab

The project information tab includes the following information:

- Name: The filename of the project
- Data Repository: the file path of the project
- Description: a long form description of the project

Project Information	Project Coordinate	Units	Model Default	s	
Name: *					
conceptual-model					
Data Repository					
	Documents\VMODFle	x\Tutoria	ls\Conceptual I	lodel	
Description:					

Project Coordinate System

The Project Coordinate tab contains a description of the project spatial reference system, which includes:

• **Coordinate System:** a systematic transformation of latitudes and longitudes of locations from the surface of a sphere or ellipsoid onto a two-dimensional plane. Supported examples include the Universal Transverse Mercator (UTM) Projection, and Lambert conformal conic (LCC) (used in the State Plane spatial reference system)

- Datum: The horizontal datum is the model used to measure positions on the Earth. A specific point on the Earth can have substantially different coordinates, depending on the datum used to make the measurement. There are hundreds of local horizontal datums around the world, usually referenced to some convenient local reference point. Contemporary datums, based on increasingly accurate measurements of the shape of the Earth, are intended to cover larger areas. The WGS84 datum, which is almost identical to the NAD83 datum used in North America and the ETRS89 datum used in Europe, is a common standard datum. Supported examples include WGS84, NAD27, NAD83, and ETRS89.
- Units: Units of length and distance. Supported examples include feet and meters.

Please Note: The project spatial reference is set when the project is created and cannot be subsequently changed. Shapefiles with a supported specified spatial reference system other than the project spatial reference system will be automatically transformed to the project spatial reference system during the import process. If the project spatial reference system is unknown or in a local or unsupported coordinate system, use the Local Cartesian spatial reference system; however, all imported data is assumed to be in the same local spatial reference system and no transformations will be applied to imported shapefiles in this case.

Project Setting				
roject Information	Project Coordinate	Units	Model Defaults	
Coordinate Systems	3: *			
SPCS83 Virginia So	outhern Zone(ft)			\sim
Datum: *				
NORTH AMERICA	N 1983, CONUS			

Units

Visual MODFLOW Flex allows you to specify which measurement units are used in your project. Measurement units are only used during model translation to convert all units into consistent base units.

Available units include the more common units in the International System of (SI) Units, informally known as the metric system, and the United States Customary System (USC) system. Please note that the imperial system of measurements is closely related to the USC, but there are differences for some units (e.g. 1.0 imperial gallons \approx 1.200 945 US liquid gallons).

Consistent Units

All of the modeling engines (e.g. MODFLOW-2000, -2005, -NWT, -LGR, -USG, -SURFACT, SEAWAT, MT3D-MS, and RT3D) rely on consistent units which are specified using the three major base units associated with groundwater flow, transport, and related processes - length (L), mass (M), and time (T). Note that the temperature units (K), which are used in heat transport simulations supported by the SEAWAT engine, are hard-coded to use degrees Celsius.

Compound Units

Compound measurement units are those measurement units that consist of combinations of base units. Examples include conductivity (L/T), recharge (L/T), concentration (M/L³), and specific storage (1/L). As discussed above, compound units are converted into consistent base units at the time of model translation. That is all compound units are converted from the specified compound units into units that are consistent with the individual base units. For example, in a project with base units of meters for length and days for time, a recharge value of 3.65 mm/yr would be converted into $1.0x10^{-5}$ m/d at translation. Note that output values with compound units (e.g. concentrations) are converted back into the specified project units when being displayed in Visual MODFLOW Flex.

Please Note: In Visual MODFLOW Flex, changing from one project unit to another will not change the magnitude of the value shown in the user interface. For example, if you change the conductivity units from ft/d to m/d, a value of 1 ft/d would be 1 m/d in the model run conductivity arrays rather than 0.3048 m/d.

Project Information Project Coordinate	Units	Model Defaults	
✓ Unit Settings			
Concentration	uç	g/L	
Conductivity		/d	
Density (includes Bulk Density)		g/m^3	
Groundwater Flow	fť	^3/s	
Length	ft		
Mass	kg	-	
Mass Flow		s/d	
Pumping Rate		PM	
Recharge		/yr	
Specific Storage		/ft	
Stream Flow		^3/s	
Temperature	°C		
Time	da	•	
Volumetric Flow	fť	^3/s	
Concentration			

Units Supported in Visual MODFLOW Flex

Measurement	t Dimensi n	o Supported	SI Units	Supported Units	
Concentration	M/L3	• mg/L • µg/L			
Conductivity	L/T	• m/s • m/d	 cm/s cm/d	● ft/s ● ft/d	
Density (including Bulk Density)	M/L3	 g/cm³ g/m³ kg/m³ 			
Groundwater Flow	L3/T	 m³/d m³/min m³/s 	 L/d L/min L/s 	 ft³/d ft³/min ft³/s 	GPMGPDMGD
Length*	L	• m		• ft	
Mass*	М	• kg • g			
Mass Flow	M/T	 kg/yr kg/d kg/hr 	 kg/min kg/s	lb/yrlb/dlb/hr	Ib/minIb/s
Pumping Rate	L3/T	• m ³ /d	• L/d	• ft³/d	• GPM

Measurement Dimensio Supported SI Units n			Supported USC Units		
		 m³/min m³/s 	L/minL/s	 ft³/min ft³/s 	GPDMGD
Recharge	L/T	 m/yr m/d	mm/yrmm/d	ft/yrft/d	in/yrin/d
Specific Storage	1/L	 1/m 1/cm		• 1/ft	
Streamflow	L3/T	 m³/d m³/min m³/s 	 L/d L/min L/s 	 ft³/d ft³/min ft³/s acre-ft/da 	 GPM GPD MGD y
Temperature*	K	• °C			
Time*	Т	• s • d • yr			
Volumetric Flov	w L3/T	 m³/d m³/min m³/s 	 L/d L/min L/s 	 ft³/d ft³/min ft³/s 	GPMGPDMGD

Note:

* Denotes a base unit

Abbreviations:

m = meter cm = centimeter mm = millimeter ft = USC survey foot

 $\mu g = microgram$ mg = milligram g = gramkg = kilogram

L = liter GPM = USC liquid gallons per minute GPD = USC liquid gallons per day MGD = million USC liquid gallons per day

s = secondmin = minute d = dayyr = year

°C = degree Celsius

Model Defaults

Model defaults are those values that will be populated into the relevant model properties on creation if no other value is specified in the development process. In other words, changing

the model default values after model values have been created will have no effect on the values in the model as these values have already been applied. Certain physical constants/material properties are also specified at this tab.

roj	ect Information Project Coordi	nate Unit	s I	Model Defaults	
	2 ↓ □				
	Bulk Density				
	Bulk Density (kg/m^3)			1700	
~	Conductivity				
	Kx (m/s)			4	
	Ky (m/s)			4	
	Kz (m/s)			0.4	
×	Constants				
	Compressibility of Air (COMPA	IR) (ft^2/lbf)		1.777E-05	
	Compressibility of Water (COM	IPWAT) (ft 2	2/lbf)	1E-08	
	Density of Air (RHOAP) (kg/ft			1.777	
	Density of Water (RHOWP) (k			1000	
	Gravitational Acceleration (GF	RAV) (ft/s^2))	9.8066	
	Standard Atmospheric Pressure (ATMGP) (bf/ft^2)			^2) 101000	
	Viscosity of Air (VISG) (b/ft.s)			1.983E-05	
	Viscosity of Water (VISW) (Pb/ft.s)			0.001	
~	Dispersion				
	Dispersion (m)			10	
v	Initial Concentrations				
	Initial Concentrations (mg/L)			0	
~	Initial Heads				
	Initial Heads (m)			100	
~	Storage				
	Effective Porosity			0.14	
	Ss (1/m)			1E-05	
	Sy			0.2	
	Total Porosity			0.3	
~	Unsaturated Zone Prope	rties			
	EPS			3.5	
	THTi			0.3	
	THTs			0.3	0.3
~	Vadose Zone				
	Brook			5	
	VANAL (m)			1	
	VANBT				
	VANSR			0.03	
Bu	ılk Density				
-			-		

2.1.2 Backup Project

The backup project dialog allows you to save your project in a compressed .zip archive, so that you can backup the currently loaded project. **Please note that you should always save your project before creating a backup.**

Backup Project	x
Backup name	
C:\Users\[user]\Documents\Visual MODFLOW Flex\Projects\[Project].zip	Browse
Include engine files	
Include companion files	
ОК	Cancel

The backup project includes the following options:

- Backup Name: path and filename for the zip file archive of your project
- **Include engine files**: the zip file will include MODFLOW and other applicable engine input and output files. Note that these are the files that are produced at the translate and run workflow steps. These files can be rather large, particularly for models with large grids and/or with many stress periods.
- Include companion files: the zip file will include all files and (sub)folders in the same directory as the current project.

2.1.3 Preferences

The preferences menu allows you to adjust various settings in Visual MODFLOW Flex:

- Flex Viewer
- <u>3D Viewer</u>
- <u>General</u>

Flex Viewer Settings

The Flex Viewer Settings include the option to select which properties are shown in the status bar and how they are formatted.

Visual MODFLOW Flex 9.0 Help

Statusbar		
Cell Properties Visibility	Decimal Places	Example
✓ Layer		
Row		
Column		
Horizontal Coordinate	#,###.00 ~	12,345.68
Vertical Coordinate	#,###.00 ~	12,345.68
✓ Width	#,###.00 ~	12,345.68
🗹 Length	#,###.00 ~	12,345.68
Thickness	#,###.00 ~	12,345.68
🗹 Area	#,###.00 ~	12,345.68
Volume	#,###.00 ~	12,345.68
Attribute	~	12345.6766321

3D Viewer Settings

The following settings are available for 3D Views in Flex:

64

🐯 Preferences		_		\times
Flex Viewer 3D Viewer General				
OpenGL Driver Use hardware accelerator Use MS Driver	Virtual Data Grid Qualty of Grid Visualization Custom Qualty	High (160)	~	
Point Style	Surface Visualization quality	1		
Basic (only sphere and cube)	Surface Quality	High (160)	~	
O Advanced (all symbols)	Custom Surface Quality			
Parallel Execution				
	ОК	Cancel	Help	

OpenGL Driver

By default, Visual MODFLOW Flex will attempt to use the vendor-provided driver included with your graphics acceleration hardware. If problems are encountered with the vendor-provided drivers, e.g., poor on-screen display/performance, Visual MODFLOW Flex provides the option to use the Microsoft Driver for OpenGL.

Virtual Data Grid

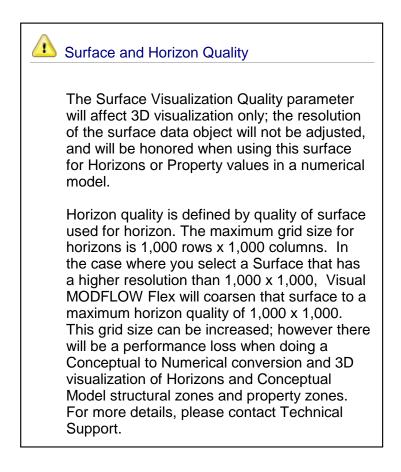
Depending on the size of your model, Visual MODFLOW Flex may run very slowly during rotations or when 3D Numerical Gridded data objects are moved in the 3D Viewer (e.g. MODFLOW Heads, Drawdown, Properties, or Transport Concentrations). In this situation, the virtual data grid option may be used to increase the speed of the data processing and image rendering. It can be used to set up a uniformly spaced grid with a specified number of rows and columns.

The virtual data grid option will interpolate the data from the model to the uniformly spaced virtual grid. This allows a smaller amount of information to be processed much faster. However, this also results in a loss of resolution of the data when viewing the data, and some local scale minimum and maximum values may be missed.

If you are experiencing performance issues, try choosing the "Low" option. The number presented in parentheses is the number of cells used along the X and Y axis for the virtual data grid.

Surface Visualization Quality

This parameter controls the visualization quality and speed of surface data objects for the 3D viewer. This parameter can be used when you want to display surfaces with a large grid size (eg. 500 x 500 or greater). Similar to the Virtual Data Grid option above, Surfaces will be resampled to the defined grid size (where the number in parentheses represents the uniform number of rows/columns).



Point Style

This setting provides two options for displaying points in 3D Viewer: Basic and Advanced. If the Basic option is selected, 3D Viewer will render the point shapes in the 3D Viewer. On some computers this option may hinder the performance of the 3D Viewer. If the Advanced option is selected, 3D Viewer will use bitmap images to display the points. If you are experiencing performance issues display points in 3D Viewer, the Advanced option should be selected.

Please Note: The Basic option only supports cube and sphere symbols for displaying points.

General Settings

The following settings are available for 3D Views in Flex:

🐯 Prefere	nces						_		\times
Flex Viewer	3D Viewer	General							
Default Dat	a Repository	•							
C:\Users\k	doerken\Doo	uments\V	isual MODF	FLOW FI	ex\Project	s		5	
Create a	a folder for th	e project							
Send A	nonymous Us	age Statis	tics						
					ОК	Car	ncel	Help)

Default Data Repository

The Default Data Repository allows you to specify a default folder location for creating new projects. The "Create a folder for the project" option allows you to specify if the new project should be added to a subfolder with the project name when the new project is created.

CAUTION: The Visual MODFLOW Flex file structure includes many managed data files, which are continuously read from and written to the project data folder. For best performance and stability, it is strongly recommended that you only save projects to local disk folder that are NOT managed by file synching/sharing services (such as OneDrive, SharePoint, DropBox, Box, etc.). These file synching/sharing services are not aware of the Visual MODFLOW Flex file structure and are not likely to not keep up with the files as they are created which will likely lead to project corruption. Saving projects over slow network connection may cause similar issues.

Anonymous Usage

By default, Visual MODFLOW Flex collects anonymous usage statistics. The data that we collect enables us (Waterloo Hydrogeologic) to get reliable statistics on which features are used (or not used). This helps us better understand the needs of our users so we can build better applications. The information collected is *anonymous* – it is not traceable to any individual, project, or organization.

You can opt out by deselecting this option. If you have additional questions about our Anonymous Usage, please email us at <u>gm@waterloohydrogeologic.com</u>.

2.2 **Project Version Compatibility**

Visual MODFLOW Flex is backwards compatible with projects made in earlier versions. However, Visual MODFLOW Flex is not forwards compatible, which means you cannot open a project that was made in a newer version of the software than you are running. This generally means that if you are working on modeling projects in a team environment, it is recommended that all members of the team work using the same version of Visual MODFLOW Flex.

Creating a full backup is strongly recommended before opening projects made in older versions of Flex, since Visual MODFLOW may update certain files during common operations without an explicit save. Please use caution when opening projects made in older versions of Flex without such a backup.

Working with older projects in Flex

From Visual MODFLOW Flex version 6.1 and onwards, the application will detect if you are using the latest version and prompt you to back up your project automatically.

Backup Project

Project backups will include a zip archive of the Visual MODFLOW Flex project files which consist of the {project_name}.amd and {project_name}.data folder. You may also optionally include the engine files and/or companion files.

Backup Project	\times
This project was created in a previous version of Visual MODFLOW Flex and will be converted to version 6.1 (build 7088), which may not open anymore in the previous version.	
Do you want to create a backup copy?	
Backup	
Project files	
Engine files	
Companion files	
Yes No Cancel	

- **Engine files**: the model input and output files associated with individual engine runs (e.g. MODFLOW-2005, MT3D-MS, ZoneBudget, MODPATH, PEST, etc.). These files can be quite large and are often easily regenerated (if you developed the entire model in Visual MODFLOW Flex), so it may be preferable to exclude these.
- **Companion files**: external files such as basemap images, DXFs, shapefiles, associated with the project but that are stored outside of the project.data folder.

2.3 Keyboard Shortcuts

The following keyboard shortcuts are available when using Visual MODFLOW Flex:

- General Shortcuts
- <u>3D-Views</u>
- Translation Step Translated Package Tabs

General Shortcuts

The following shortcuts are applicable at when the main window is open and active:

Command	Shortcut	Description/Result
Help Topics	F1	Opens the built-in help documentation including tutorials and getting started guides
New Project	CTRLN	Opens the Create New Project setup dialog

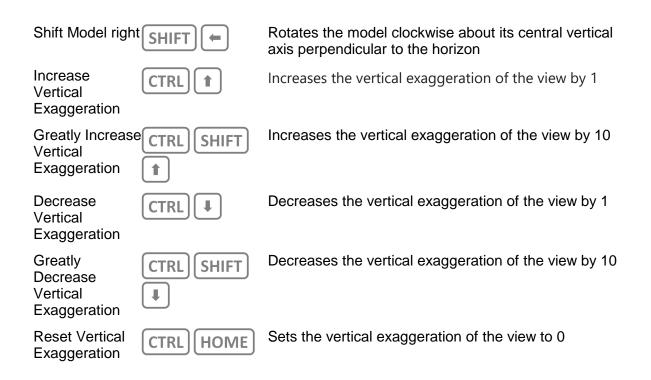
Visual MODFLOW Flex 9.0 Help

Open Project	CTRLO	Opens an existing project
Import Project	CTRL	Imports a Visual MODFLOW Classic (*.vmf) file
Save Project	CTRLS	Saves the active project to its current location; except at the Translation workflow step where the shortcut saves the active package file
Save Project As	s F12	Saves the active project in a selected location
Import Data	CTRLD	Opens the Import Data dialog to add external data to your project
Exit	ALT F4	Exits Flex - you will be prompted to save your project if one is open
Workflow Tree	F4	Shows/hides the workflow tree for the active workflow
Model Explorer	F11	Shows/hides the model explorer/data explorer panel

3D-Views

The following shortcuts are applicable at when a 3D-Viewer is active (i.e. its title bar is shown in blue)

Command	Shortcut	Description/Result
Shift Model up		Shifts the model up in the viewer relative to the viewer window
Shift Model down	Ŧ	Shifts the model down in the viewer relative to the viewer window
Shift Model left	\Rightarrow	Shifts the model left in the viewer relative to the viewer window
Shift Model righ	t 🗲	Shifts the model right in the viewer relative to the viewer window
Reset Model View	HOME	Re-centers the 3D View to the model centroid and the view/rotation angle to directly above the model and aligned North
Rotate towards horizon	SHIFT	Rotates the foreground of the model upwards about its central axis parallel to the horizon
Rotate model away from horizon	SHIFT	Rotates the foreground of the model downwards about its central axis parallel to the horizon
Shift Model left	SHIFT -	Rotates the model counter-clockwise about its central vertical axis perpendicular to the horizon



Translation Step - Translated Package Tabs

The following shortcuts are applicable at when a translated package tab is active at the Translation Workflow Step:

Command

Shortcut

Description/Result

Save Edits



Saves text edits to the active translated file

3 Quick Start Tutorials

The following tutorials provide a brief introduction on how to use Visual MODFLOW Flex. The objective is not to teach you every detail, but to familiarize you with basic principles and the way the program works. The steps are intentionally kept brief so that you can actually start using the program as quickly as possible. You are encouraged to explore the more detailed sections of the Help documentation to further familiarize yourself.

In Visual MODFLOW Flex, there are two workflows you can follow: Conceptual or Numerical Modeling. Please take a moment to review the summary below to help you decide where you should start.

Conceptual Modeling (Recommended for Creating New Models)

Use this option if you want to:

- Start a new modeling project and have various data types/formats (GIS etc.) for defining the geological layering, material properties, and boundary conditions;
- Simulate domains with complex geological layering (pinchouts and discontinuities);
- · Evaluate multiple numerical grids for your project; or
- Work with unstructured grids

The Conceptual Modeling tutorial will walk you through the following steps:

- Loading your raw data
- Defining the Geological Structure
- Defining the Properties and Boundaries
- Defining a Grid or Mesh
- Converting this to a Numerical Model

Start the Tutorial!

Numerical Modeling (For Existing Models)

Use this option if you want to:

- Create a MODFLOW-based numerical model (define the numerical grid and populate the grid the properties and boundary conditions; similar to conventional Visual MODFLOW);
- Import a Visual MODFLOW project set (*.VMF); or
- Import a standard USGS MODFLOW data set (MODFLOW-2000, -2005)

Start the Tutorial!

See Also:

Several sample projects are available for download from our <u>tutorial webpage</u>, that illustrate both the conceptual and numerical modeling workflows.

3.1 Conceptual Modeling Tutorial

The following example is a quick walk-through of the basics of building a conceptual model and converting this to a numerical model.

Objectives

- Learn how to create a project and import your raw data
- · Become familiar with navigating the GUI and steps for conceptual modeling
- Learn how to define a 3D geological model and flow properties
- Define boundary conditions using your GIS data
- Define a MODFLOW grid, then populate this grid with data from the conceptual model
- View the resulting properties and boundary conditions
- Translate the model inputs into MODFLOW packages and run the MODFLOW engines
- · Understand the results by interpreting heads and drawdown in several views
- Check the quality of the model by comparing observed heads to calculated heads

Required Files

Several files are required for this exercise, which should be included with the Visual MODFLOW Flex installation.

These files are available in your public "My Documents" folder, typically:

C:\Users\Public\Documents\Visual MODFLOW Flex\Tutorials\Conceptual Model\supp files

If you cannot locate these files, please download them from our website.

Creating the Project

Launch Visual MODFLOW Flex



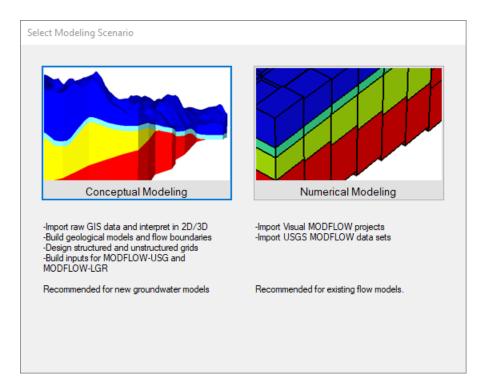
- Select [File] then [New Project...]. The Create Project dialog will appear.
- Type in project name 'Conceptual Modeling Tutorial'.

- Click the [^[]] button in Data Repository field, navigate to a folder where you wish your projects to be saved, and click **[OK]**.
- Click the 'Create a folder for the project' checkbox
- Define your coordinate system and datum (or leave the default value Local Cartesian).
- For this project, the default units will be fine.

The Create Project dialog should now look like this (ensure the units are the same):

😂 Create Project				?	\times
Project Information	Units *				
Name: *	● ● Z				
Conceptual Modeling Tutorial	V U	nit Settings			
		oncentration	mg/L		
Data Repository: *	Co	onductivity	m/s		
C:\Users\bconicelli.WH\OneDrive - Waterloo Hydrogeok	De	ensity (includes Bul	k De kg/m^3		
		oundwater Flow	m^3/d		
Create a folder for the project	Le	ngth	m		
Desertetions		ass	kg		
Description:	M	ass Flow	mg/yr		
	Pu	Imping Rate	m^3/d		
	Re	echarge	mm/yr		
	Sp	ecific Storage	1/m		
	St	ream Flow	m^3/d		
	Te	emperature	°C		
		me	day		
Project Coordinate	Vo	olumetric Flow	m^3/d		
Coordinate Systems: *					
Local Cartesian					
Datum: *	Conc	entration			
World Geodetic System 1984					
		ОК	Cancel	Н	elp

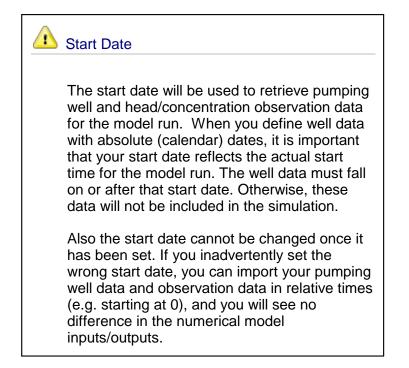
• Click **[OK]**. The workflow selection screen will appear.



- Select [Conceptual Modeling] and the Conceptual Modeling workflow will load.
- In the Define Modeling Objectives step, you define the objectives of your model and the default parameters.

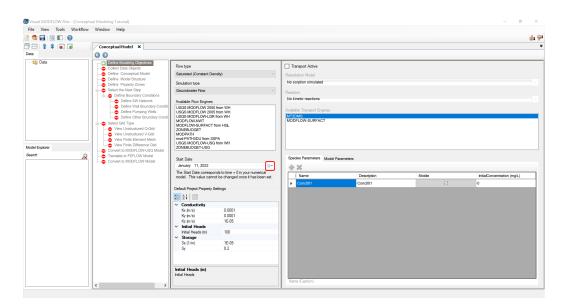
File Vert Noti Window Help Image: Section Planeters Image: Section Planeters Image: Section Planeters Image: Section Planeters Section Planeters Section Planeters Model Explorer Convert to MCO/CL/V/SIG Model Section Planeters Section Planeters Convert to MCO/CL/V/SIG Model Section Planeters Model Explorer Section Planeters Model Planeters Model Explorer The Sall Bale Decomposition Bale Planeters Model Planeters Model Explorer Model Planeters Model Planeters Model Planeters Model Planeters Model Planeters	Visual MODFLOW Flex - [Conceptual Modeling Tutorial]				- 0	×
Image: Conceptent Hold IX Data Image: Conceptent Hold IX Image: Concent Hold IX <td< th=""><th>File View Tools Workflow Window Help</th><th></th><th></th><th></th><th></th><th></th></td<>	File View Tools Workflow Window Help					
Des Image: All of the second	2 🍓 🕞 🔢 🗈 👔				4	a 🗭
Constrained of Constrained Constrained Constrained Constrained Constrained Constrained Constrained Constrained Constrained Constrained Constrained Constrained Co	Conceptual Model X					Ŧ
Model Explore Control to Conjugation File type Product Note Model Explore Outrie Thread Difference Organization (See Organization (Data (3 6)					
Default Proget Program Image: Proget Program Image: Proget Pr	Date Date Date	Sexual (Constant Density) - Simulation hole - Consulvater fine - Analaka Flow Expanse - USGS MODELCW 2000 hem VH - USGS MODELCW 200 hem VH - USGM 2000 hem VH - VERSUBARD 20000 hem VH	Petadation Model No softon simulated Peaction No kinetic reactions MOOFLOW-SURPACE MOOFLOW-SURPACE Name Name MOOFLOW-SURPACE Name Name Name Name Name Name Name Name	Description		

• The **Start Date** of the model corresponds to the beginning of the simulation time period. It is important to define a relevant start date since your field measurements (observed heads and pumping schedules) will be defined with absolute date measurements, and must lie within the simulation time period. For this scenario, the default objectives will be fine.



Setting the Start Date

The model start date for this exercise should be set to **1/1/2000**. Visual MODFLOW Flex uses a standard Windows date picker; a few tips are shown below on how to use this. Click on the button shown below, to load the Windows date picker.



The standard Windows calendar will appear. Click on the month in the header (as shown below):

•	- (Nove	ember	2020		►
Sun	Mon	Tue	Wed	Thu	Fri	Sat
25	26	27	28	29	30	31
1	2	3	4	5	6	7
8	9	10	11	12	13	14
15	16	17	18	19	20	21
22	23	24	25	26	27	28
29	30	1	2	3	4	5
Today: 11/16/2020						

All months for the current year will appear as shown below. Click on the year in the header:

4	20	20	•		
Jan	Feb	Mar	Apr		
May	Jun	Jul	Aug		
Sep	Oct	Nov	Dec		
Today: 11/16/2020					

A range of years will then appear as shown below. Click on the range of years in the header:

4	2020-	2029	•		
2019	2020	2021	2022		
2023	2024	2025	2026		
2027	2028	2029	2030		
Today: 11/16/2020					

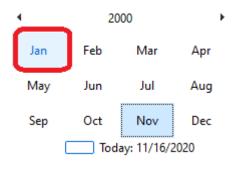
A list of years for the previous decade will appear. You can then use the < or > buttons to change the year. Select the 2000-2009 period:

4	2000-	×		
1990-	2000-	2010-	2020-	
1999	2009	2019	2029	
2030-	2040-	2050-	2060-	
2039	2049	2059	2069	
2070-	2080-	2090-	2100-	
2079	2089	2099	2109	
Today: 11/16/2020				

Once you have reached the desired decade, select '2000' on the calendar as shown below:



A list of months will then appear for that year. Select January for this example, as shown below:



Finally, select "1" from the calendar as shown below:

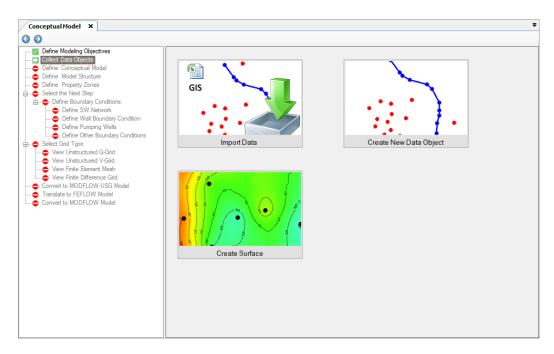
4		Jan	uary 2	000		•
Sun	Mon	Tue	Wed	Thu	Fri	Sat
26	27	28	29	30	31	1
2	3	4	5	6	7	8
9	10	11	12	13	14	15
16	17	18	19	20	21	22
23	24	25	26	27	28	29
30	31	1	2	3	4	5
		1	loday:	11/16/	/2020	

The selected date (January 1, 2000) will then appear for the Start Date.

- For this scenario, the remainder of the default objectives and values will be fine.
- Click [(Next Step) to proceed.

Collect Data Objects

• The next step is to import or create the data objects you will use for building the conceptual model.



At this step, you can import data, create new data objects (by digitizing) or create surfaces (from points data objects)

• Click the [Import Data] button and the following screen will load:

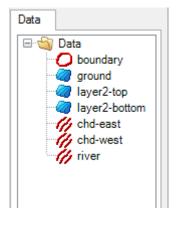
*	Data Import		- 🗆 ×
Data Source			
Data Type: *			
Point			¥
Source File: *			
Name: *			
Description			
Description:			
		< <back next="">></back>	Cancel Help

• Select Polygon in Data Type combo box.

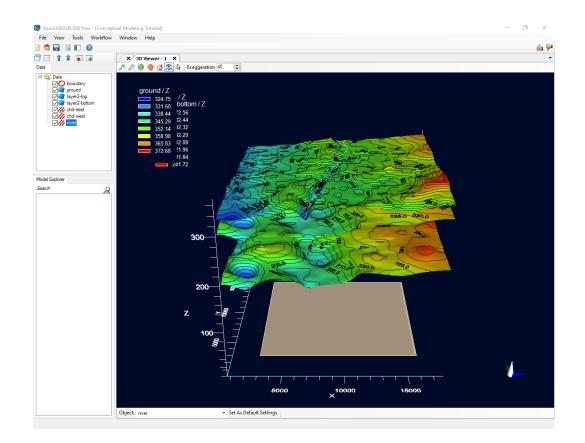
 In the Source File field click the [...] button and navigate to your 'My Documents' folder, then 'Visual MODFLOW Flex\Tutorials\Conceptual Model\supp files', and select boundary.shp.

Please Note: The files may be located in the public documents folder: "C: \Users\Public\Documents\Visual MODFLOW Flex\Tutorials\Conceptual Model\supp files", if you selected to make the program available to all users on install.

- Click [Next>>].
- Click [Next>>].
- Click [Next>>] then Click [Finish].
- The next step is to import a surface that represents ground surface.
- Click the [Import Data] button.
- Select **Surface** for the Data type.
- In the Source File field click the [...] button and navigate to the 'My Documents' folder, then 'VMODFlex\Tutorials\ConceptualModel\supp files' folder, and select ground.grd.
- Click [Next>>] through all the screens to accept the defaults, then click [Finish].
- Repeat these steps to import the remaining Surfaces: layer2-top.grd, layer2bottom.grd.
- Next, import polyline data objects, and from the same source directory ,select chdeast.shp; use all the defaults and finish the import.
- Repeat these steps, for polylines, importing first **chd-west.shp**, then **river.shp**.
- Once the data objects are imported, they will appear in the tree on the left side of the program window.



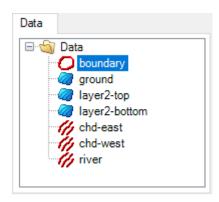
- You can view these data objects in 2D or 3D; simply create a new viewer:
- Click on [Window] then [New 3D Window] from the main menu; an empty 3D Viewer will appear;
- Click on the check box beside each of the data objects you imported, and they will appear in the 3D Viewer.
- Increase the vertical exaggeration and use the mouse to reorient the screen so that you can see all your data objects, as in the image below.



- Close the 3D View by clicking on the "X" of the $\sqrt{3D \text{ Viewer 1}} \times |$. tab
- On the Conceptual Model tab click [[(Next Step) to proceed, where you will arrive at the Define Conceptual Model step.

Define Conceptual Model

- Provide a name for the conceptual model (e.g. Conceptual Model 1), and model area.
- From the Data Explorer, select the polygon data object called "boundary" (which represents the horizontal extents of the conceptual model) so that it is highlighted:



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• Click the [] button in the Model Area to insert it as the reference object in the Define Conceptual Model workflow step.

Save	
Name *	
Conceptual Model 1	
Description	
Model Area	
Select existing data object	
boundary	
Projection Type	
Coordinate Systems: *	
Local Cartesian V	
Datum: *	
World Geodetic System 1984	

Please Note: The model area cannot be defined using a complex polygon (a polygon that intersects with itself) or with a polygon data object that contains multiple polygons.

• Click **[Save]**. Notice that the conceptual model elements have been added to the Model Explorer tree in the lower left section of the application window.

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• Click [] (Next Step) to proceed to the Define Model Structure step.

Define Structure

Defining the geological model consists of providing geological surfaces as inputs for horizons. Then three-dimensional solids are created between these horizons. To create new horizons, follow the steps below.

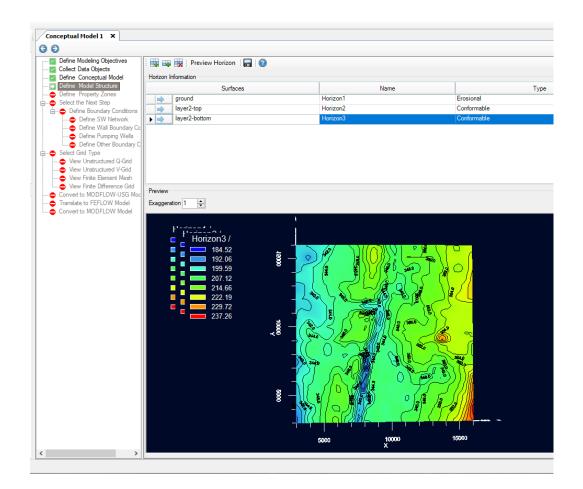
- From the Horizons Settings dialog (shown below), click the [Herizon] button to add a new horizon row to the Horizon Information table.
- Repeat this two more times so there are 3 new rows on the Horizons table.
- From the Data Explorer, select the **ground** surface data object that will be used to generate the horizon
- Click the []] button in **Row1** of the Horizons grid, to insert it into the Horizon Information table. See the example below.

Conceptual Model 1 ×			
G Ð			
Define Modeling Objectives	👯 共 🙀 Preview Horizon 🛛 📊 📀		
Define Conceptual Model	Horizon Information		
Define Model Structure	Surfaces	Name	Туре
Define Property Zones	ground	Horizon1	Erosional
- Select the Next Step		Horizon2	Conformable
🚊 😄 Define Boundary Conditions			
Define Wall Boundary Cc		Horizon3	Conformable
Contraction of the second secon			
Define Boundary Conditic			
Select Grid Type			
View Unstructured Q-Grid			
View Unstructured V-Grid			
View Finite Element Mesh			
View Finite Difference Grid			
Convert to MODFLOW-USG Moc			

- For this example, the default horizon type will be adequate. For an explanation of each horizon type, please refer to the "<u>Horizon Types</u>" section of the user manual.
- Repeat the steps above to add additional horizons:
- From the Data Explorer, select the layer2-top surface data object, click the [button in Row2 of the Horizons grid, to insert it into the grid.
- From the Data Explorer, select the layer2-bottom surface data object, click the [button in the Row3 of Horizons grid, to insert it into the grid.

Please Note: Horizons are added in order from the topmost geological contacts and working downwards.

- You can preview the horizons in the adjacent 3D Viewer by clicking the [Preview Horizon] button.
- Once finished, you should see a display similar to the one shown below.



- Click the [] [Create and Save] button to generate the model horizons, you should see them populate into the Model Explorer.
- Finally, click the [] button to proceed to the next step (clicking the [] will also automatically generate the model horizons in the Model Explorer, if you didn't already click the [Create and Save] button).

Define Property Zones

Once you have imported sufficient raw data into your project, you can begin to construct one or more conceptual models using imported or digitized data objects as building blocks.

At this step, you can view/edit the flow properties for the model. There are two ways to define property zones: Using Structural Zones, or Using Polygon Data Objects. For this tutorial, we will use the structural zones.

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Using Structural Zone(s)

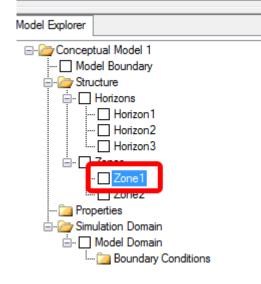
This method allows you to generate property zones using the structural zones generated in the Define Model Structure step.

• Click on the [Use Structural Zone] button as shown below

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		Zone Metho ructural Zon rgon Data O	e(s)	Sele	Struc	tore stru tural Z	uctural zone ones	s	Property Zones Property Zone 1
Name									
Property	y Zone 1								
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	Kx	m/s	Constant		0.0001		Object	¥	

• Select **Zone1** structural zone from the conceptual model tree (under the Structure/Zones node as shown below)



• Click the []] button to insert the zone in the Structural Zones field, as shown below.

Crea	te New Property	Zone Metho	d	Se	ect one or m	nore stri	uctural zone	s	Property Zones
	Use St	ructural Zone	e(s)	*					Property Zone 1
	Use Poly	rgon Data Ol	bject	•0		tural Z	ones	_	
Name)								
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	Parameter	Unit	Method		Value		Object	Mapping	
•	Kx	m/s	Constant	~	0.0001	⇒		×	
	Ку	m/s	Constant	~	0.0001	•		×	
	Kz	m/s	Constant	~	1E-05	•		¥	

- Select the Group of parameters that will be defined, e.g., Conductivity, Storage or Initial heads. The data input grid below will display the appropriate parameters based on which parameter group is selected. For example, if conductivity is selected, the data input grid will show the parameters Kx, Ky, and Kz. The data input grid will already be populated with the default values specified in the Project Settings (accessible from the main menu by clicking File > Project Settings...).
- **Type** the following values for the property zone 1: **Kx = 4E-6**, **Ky = 4E-6**, **Kz = 4E-7**)

Prope	rty Values							
Group	of parameters t	o define						
Cond	uctivity (Kx, Ky,	Kz)	~					
	Parameter	Unit	Method		Value		Object	Mapping
•	Kx	m/s	Constant	~	4E-06	₽		×
	Ку	m/s	Constant	~	4E-06	•		×
	Kz	m/s	Constant	~	4E-07	€		×

- Click on the [Save] button located on the right side of the window.
- Repeat these steps for the other property zone:
- Click on the [Use Structural Zone] button
- Select Zone2 from the model tree
- Click on [] button to insert the zone in the Structural Zones field, as shown below.
- Type the following values for property zone2: Kx = 7E-5, Ky = 7E-5, Kz = 7E-6
- Click on the [Save] button located on the right side of the window.

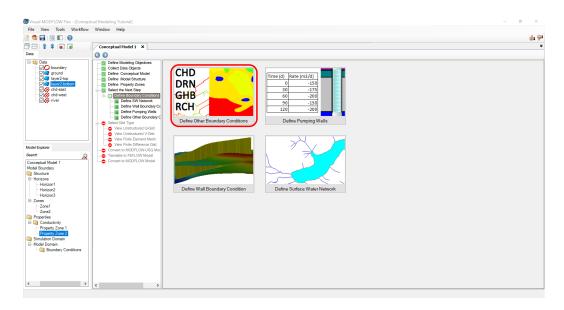
Create	e New Property	Zone Meth	od			iore stru	uctural zone:	S	Property Zones Property Zone 1
	Use Str	ructural Zon	ie(s)	÷₿	- 44				Property Zone 2
	Use Poly	rgon Data C)bject		Struc	tural Z 2	ones		
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	uctivity (Kx, Ky,	K-1	~						
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Condu	Parameter	Unit	Method		Value		Object	Mapping	
Condu •				~	Value 7E-05	•	Object	Mapping	
	Parameter	Unit	Method	~		+	Object		
	Parameter Kx	Unit m/s	Method Constant	_	7E-05		Object	~	

- Property zones can also be defined using polygon shapes; the values can also be defined from shapefile attributes or 2D Surface (distributed values). For more details, please see <u>Defining Property Zones</u>
- Click [[(Next Step) to proceed to the Selection screen.
- Click the [Define Boundary Conditions] button to proceed.

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In this window, you can choose the type(s) of Boundary Conditions to create: Standard MODFLOW Boundary Conditions (CHD, DRN, RCH, etc.), Pumping Wells, or Walls.

• Click on the [Define Other Boundary Conditions] button:



• The Define Boundary Condition dialog box will appear on your screen as explained in the following section.

Define Boundary Conditions

- At this step, you can define flow boundaries for the model.
- From the **Select Boundary Condition Type** combo box, select the desired boundary condition type.
- Select 'Constant Head (Type 1)'
- Type name: 'Constant Head East'.
- From the Data Explorer, select the **chd-east** polyline that represents this constant head.
- Click the [] button in the Define Boundary Condition dialog, to add this polyline to the input.

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oundary Condition		0
Select boundary condition type Constant Head (Type 1) Name: Constant Head East Description:	 Help Choose the desired boundary condition type from the list, and define a name and optionally, a description. Define where the boundary condition object should be connected on the simulation model domain; this will determine to what model layer the boundary condition will be translated (Top, Bottom, Intermediate). You must then select a polygon or polyline to define the boundary condition geometry. Select the Sides option if you wish to define a boundary condition to the side face of the simulation model domain. For this option, supported boundary condition types are Specified Head, General Head, and Specified Flux 	Show >>
Where to connect on the Simulation Model Domain Top Geometry Select a polyline or polygon from Data Explorer Chd-east	✓	
	<< Back Next >> Cance	Help

• Click the [Next] button.

2	Define Bound	lary Condition	n – 🗆	×
Boundary Condition				
Polylines Zones Polyline0 Image: Polyline0.Zone0 Image: Polyline0.Zone0 Image: Polyline0.Zone0	A Po	ints int1	Show Select how the attributes are defined Define for the entire zone. Apply To All Define values at vertices (Linear Interpolation) Just start and end points. All vertices.	>>
Starting Head (m)		Ending Head (m))	
Static	Ý	Static		~
Constant	~	Constant		~
347		347		
	From 3D gridded F	rom shapefile	From time schedule Transient data From Surface	
			<< Back Finish Cancel Hel	p

- The next dialog allows us to define the constant head value. Visual MODFLOW Flex provides various options for defining boundary condition attributes. Attributes can be assigned from those stored in Surface, Time Schedule, Shapefile and 3D Gridded data objects. You can also set attributes as Static (no change over time) or Transient (changes over time).
- For this tutorial, you will assign a static constant head value.

- In the empty fields located below the 'Starting Head (m)' and 'Ending Head (m)' fields type '347'.
- [Finish] button

Repeat these steps to define the other constant head boundary condition:

- Click on Define Boundary Conditions directly in the workflow tree
- Select the [Define Other Boundary Conditions] button.
- Choose Constant Head, select the chd-west polyline, and define a value of 325 for both the Starting Head and Ending Head
- Click [Finish].

Before you proceed, you will define one more boundary condition, a River.

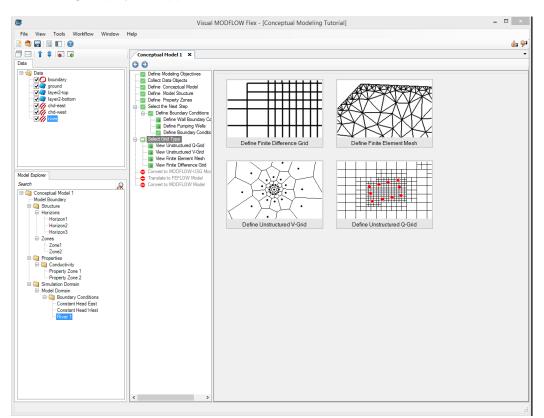
- Click on **Define Boundary Conditions** in the tree, and select the **[Define Other Boundary Condition]** button.
- Choose River (Type 3 MODFLOW Only) for the boundary condition type
- From the Data Explorer, select the river polyline
- Click the [] button in the Define Boundary Condition dialog, to add this polyline to the input.
- A warning may appear about clipping the polyline; click [OK] to continue
- Click the [Next>>] button.
- Define the following attributes for the river, as shown below: Stage = 335 (m), Bottom = 333 (m), Riverbed Thickness = 1 (m), Width = 10 (m), Riverbed conductivity = 0.01 (m/s).

>				Define Bound	lary Conditio	n				- 🗆	×
Boundary Condition											
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Stage (m)		Bottom (m)		Leakance (1/day)	Riverbed Thickr	ness (m)	River Wid	th (m)	Riverbe	d Conductivity	
Static	~	Static	~	Static V	Static	Ý	Static	~	Static		¥
Constant	~	Constant	~	Calculated V	Constant	Ý	Constant	~	Constant	t	~
335		333		\$K/\$RBTHICK	1		10		0.01		
				From 3D gridded F	rom shapefile	From time	schedule	Transient data	3	From Surface	;
						<<	Back	Finish	Cance	l He	lp

- Click [Finish].
- The River conceptual boundary condition will be added to the model tree.

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• The following display will appear.



Next you can choose what kind of grid to create:

- Define Finite Difference Grid: for a MODFLOW-6, MODFLOW-2000, -2005, or MODFLOW-LGR model run;
- Define Finite Element Mesh: for preparing inputs for a FEFLOW .FEM file;
- *Define Unstructured V-Grid*: for a MODFLOW-6 or MODFLOW-USG run with a Voronoi grid; or
- Define Unstructured Q-Grid: for a MODFLOW-6 or MODFLOW-USG run with a Quadtree grid.
- Click the [Define Finite Difference Grid] button and the following window will appear; define the inputs as explained in the following section.

•			Define I	Nume	rical	Grid								- "	
Name			_												
NumericalGrid		Add Data Object	_												
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0									 						
Grid Size					\vdash	++	\rightarrow		+		\vdash	+			
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20	650.000														
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X Min	X Max	Width			\vdash	++					++		_		
3000.000	16000.000	13000.000			\vdash	++	++		+		++		+	\square	
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3000.000	16000.000	13000.000													
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Define Finite Difference Grid

- Enter a unique Name for the numerical grid. This name will appear in the Conceptual Model tree once the grid is created.
- Enter the grid size, and optionally, the grid rotation. The grid can be rotated counterclockwise about the grid origin by entering a value between 0 and 360 in the Rotation text field.
- The Xmin and Ymin values refer to the X-Y coordinates of the bottom-left corner of the numerical grid. The Xmax and Ymax values refer to the X-Y coordinates of the top-right corner of the numerical grid.
- The Columns and Rows fields allow you to define the Grid Size.
- **Type '100'** for both the # rows and columns
- Row and Column height/width will be automatically resized based on the grid extents and number of rows/columns, as shown below:

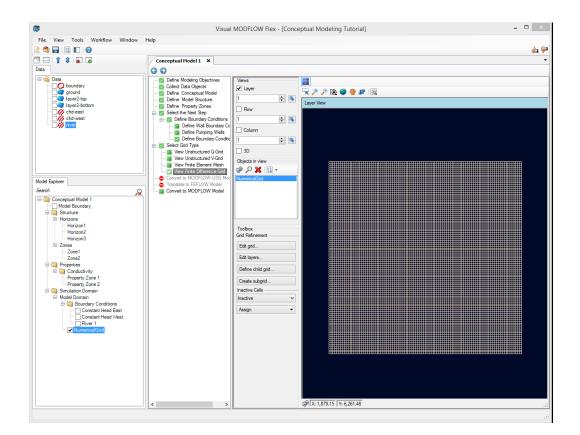
			Define Numerical Grid -	
Name				
NumericalGrid		Add Data Obj	ject	
Rotation (deg	rees)			
0				
Grid Size				
Rows	Cell Height			
100	130.000			
Columns	Cell Width	_		
100	130.000			
Grid Extents				
X Min	X Max	Width		
3000.000	16000.000	13000.000		
Y Min	Y Max	Height		
3000.000	16000.000	13000.000		
			< <back next="">></back>	Cancel

- Click the **[Next>>]** button to proceed to define the vertical discretization. You will then see a cross-section preview of the grid.
- By default, the vertical exaggeration is 1. Locate the 'Exaggeration' value below the preview window, and **type '40'** for the exaggeration value, then click **[Enter]** on your keyboard.

3	Define Numerical Grid – 🗆 🗙
Define Vertical Grid Grid Type Deformed Create Child Grid Description In a deformed grid/mesh, the tops and bottoms of the model layers follow the horizons elevations. You can refine the model layers, by dividing the zones into proportionately thick layers. Zmin 184.524382230466 Zmax 0.1	
Layer Name Layer Refinement Zone1 Zone2 Apply	Exaggeration 40 1 Column 1 +
	< <back cancel<="" finish="" td=""></back>

- In the 'Define Vertical Grid' screen, specify the type of vertical discretization
- For this exercise, the default **Deformed** grid be used.
- More details on the grid types can be found in the "<u>Defining Grids/Meshes</u>" section of the manual.
- Leave the defaults as is; click the [Finish] button.
- The grid will then appear as shown in the following screen.

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Please note: if the grid does not appear, click the show/hide gridlines button (IIII) which toggles the visibility of the grid.

• Click [] (Next Step) to proceed.

Convert to Numerical Model

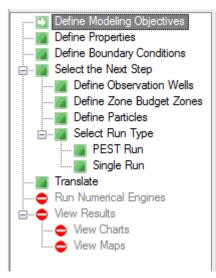
Now you are ready to populate the numerical grid/mesh with the conceptual elements.

- Click on the [Convert to Numerical Model] button to proceed
- This conversion could take several minutes, depending on the size and type of grid you used, and the complexity of the conceptual model inputs.
- A new window displaying the conversion progress will open. You should see a message indicating that the model conversion has completed. Click [Close] to dismiss this window.

Conversion Progress

Converting Prop		Property Zone 1	the layer number is: 1
Converting prop Converting prop	erty for conductivity erty for conductivity	Property Zone 1, Property Zone 2,	the layer number is: 2 the layer number is: 1 the layer number is: 2
*****Converting I Constant Head I	Boundary Conditions: East		
Constant Head River 1 ****** Conceptual	West model to numerical r	nodel conversior	has completed *****

• A new workflow tab (Numerical Modeling) will open in your project with these steps:



• Keep the default modeling objectives and click [(Next Step) to proceed to the Define Properties step.

Define Properties

• At this step, you can view/edit the flow properties for the model.

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- Under Views, select the various views you want to see in the Flex viewer; Visual MODFLOW Flex allows you to simultaneously show a layer, row, column and 3D Views. Place a checkbox beside the desired view and it will appear on screen.
- Adjust a specific layer, row, or column using the up/down arrows. Alternatively, click

on the [>] button then click on any specific row, column, or layer in any of the 2D views, and the selected row, column, or layer will be set automatically.

- Now you will define a default initial heads value.
- Choose [Initial Heads] from the combo box under the Toolbox as shown below

Views
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- Click [Edit...] button located below the Initial Heads combo box.
- Type '350' in the top 'Initial Heads (m)' cell.
- Then press **[F2]** (or the **[**^{III}] button) to propagate this value to all other cells in this column; this will apply an initial head value of 350 for the entire model domain.
- Click [OK] when you are finished.
- Use the same tools as described in the previous step to manipulate the views.
- The display tools located above the grid viewer window allow you to switch from discrete cells rendering to color shading/contours.

Please Note: this is available only when you do attribute rendering, and not when you are rendering by ZoneID

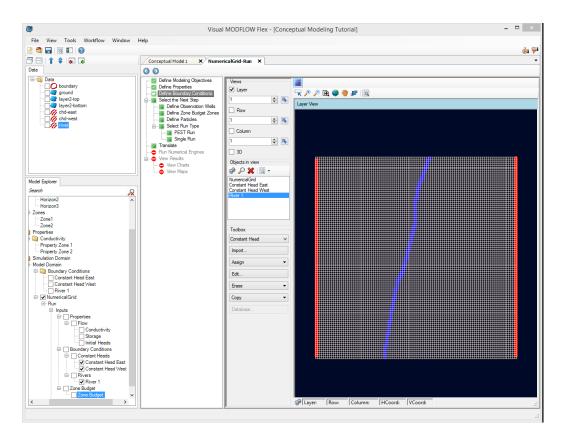


Show/hide grid lines Show as cells Show as Surface

- In the Toolbox, you can select a different parameter group and see the corresponding zonation in the Flex Viewers. For example, try turning on the column view and switching to Conductivity to see the two zones you defined earlier.
- Click [[(Next Step) to proceed to the Define Boundary Conditions step.

Define Boundary Conditions

At this step, you can view/edit the flow boundaries for the model.



- From the Objects in view window, select the Desired Boundary condition group (Constant Head, Rivers, etc..).
- Then select [Edit...].
- Click on a cell that belongs to this group; a dialog will appear where you can see the values for the boundary you selected.
- Click **[OK]** to close the view.
- Click [] (Next Step) to proceed. You will arrive at the 'Selection' step.

Proceed to Run or Define Optional Model Elements

You will arrive at a choice screen; here you can add optional/supplementary model inputs for the model that are not necessarily required to run a groundwater model simulation, including defining:

- Zone Budget Zones,
- Particles for Particle Tracking,
- Observation Wells for model calibration

Or, you can proceed directly to Running the simulation.

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• Click the **[Select Run Type]** button to proceed (Mouse over this and you will see the blue "Next" arrow appear on top; just left click once to select this option. (Alternatively,

the [[[Next step) button will take you to this step, as it is pre-defined as the default step.

Conceptual Model 1 × Numeri	calGrid-Run ×		
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View Results View Charts View Maps	Single Run	PEST Run	

- Click the **[Single Run]** button to proceed (Alternatively, the **[Single Run]** (Next step) button will take you to this step).
- You will arrive at the **'Select Engines'** step. Here you can choose what engines you want (what version of MODFLOW: 2000, 2005, etc..), and if you want to include MODPATH and ZoneBudget in the run.

USGS MODFLOW 2005 from WH	~
USGS MODFLOW 2000 from WH USGS MODFLOW 2005 from WH	_
MODFLOW-6	
USGS MODFLOW - LGR from WH MODFLOW-NWT	•
MODFLOW-SURFACT from HGL	
Particle Tracking	

- MODFLOW-2005 should be selected by default.
- Click [] (Next Step) to proceed.

Translate Packages

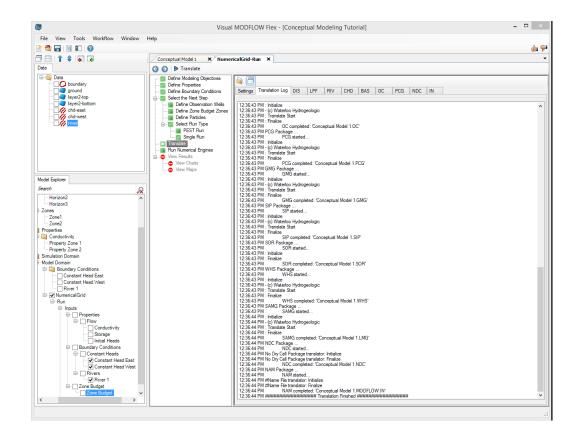
• You will arrive at the 'Translation Step'.

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At this step, you choose if the model is steady-state or transient, choose the solver you want to use, and define any other MODFLOW package/run settings, such as cell-rewetting, etc.

Please Note: in the General Settings, there is a default location indicating where the MODFLOW and related files will be generated.

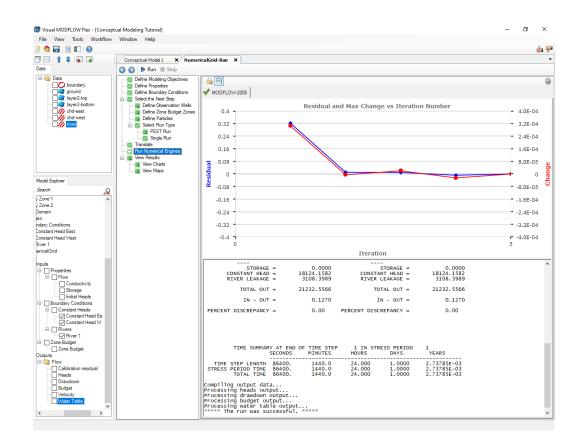
• Click the [Translate] button near the [] button to proceed; this will read the input from the numerical model and "translate" this into the various input files needed by MODFLOW and the other engines. The files will be created in the directory defined in the previous step.



• Click the [] (Next step) button to proceed. You will arrive at the "Run Engines Step".

Run Engines

• Click the [Run] button near the [] button on the main workflow toolbar to start running the engines. You will see the Engine progress presented in a chart in the top half of the screen and as text in the scrolling window below:

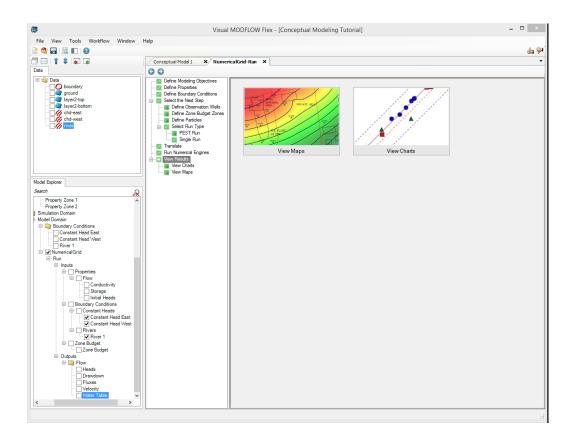


Please Note: after a successful run, the Heads (and other applicable output items) will be added the tree in the Model Explorer tree in the lower left of the application window.

• Once finished, Click the [] (Next step) button to proceed.

View Results

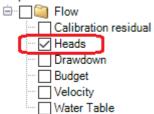
• You can then choose to view results in the form of Maps (Contours and Color shading) or Charts



- Click the [View Maps] button.
- Hit **F4** to hide the Workflow tree and make more viewing area for the maps.

Please Note: you can turn the workflow tree back on by hitting F4 at any time.

- Make sure in views you only have Layer checked "on". By default, the maps always show heads first. You can change this by checking one of the other output options in the Model Explorer:
- Outputs



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- You can see color shading of the calculated heads, in layer view.
- You can display heads along a row, and along a column, and in 3D, using the same tools as you used earlier (refer to <u>View/Edit Properties</u> section).
- If your model is transient (this exercise does not apply), you can use the time controls above the Flex Viewer to change the output time; as you do this, all active viewers (layer, row, column, 3D), will refresh to show the heads for the new output time.



• The next section will discuss how you can generate a new grid with a different size and resolution, and generate a numerical model using this grid.

Evaluating Different Grids

In some cases, the initial grid size you defined may not be adequate to provide the solution resolution you require from your model. In this section, we explain how you can generate multiple grids from the conceptual model and run the corresponding numerical models.

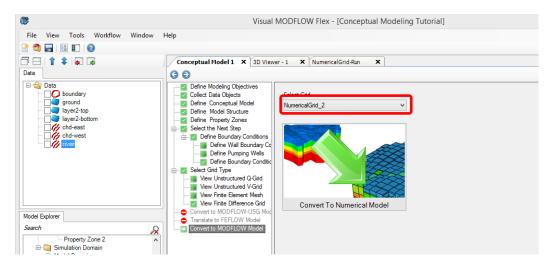
• At the top of the grid view you will see a list of active tabs:

Conceptual Model 1	х	3D Viewer - 1	×	NumericalGrid-Run	х	

- Click on the first tab, which should be your Conceptual Model workflow to make this the active window, and it should now appear on your display.
- Click [Select Grid Type] from the workflow tree.
- Click [Define Finite Difference Grid] button and the Define Grid window will appear.
- Define a new grid with the desired grid size and rotation. (try a grid with twice as many rows and columns; i.e. 200 rows and 200 columns)
- Click [Next>>].
- Specify the desired vertical discretization; you may wish to use a different vertical grid type, or refine any of the vertical layers.
- Click [Finish] when you are done.
- The new grid should now appear, and you will also see the grid appear as a new node in the Model Explorer tree.
- Click the [] (Next step) button to proceed.

Now you are ready to populate the numerical grid/mesh with the conceptual elements. The 'Convert to Numerical Model' display should appear similar as below. Now, in the 'Select Grid' combo box, you will see there are 2 grids; by default, the grid you just created should be selected.

• Click on the [Convert to Numerical Model] button to proceed.



• After clicking on the conversion button, a new workflow window will appear which includes the steps for the numerical model for this new grid.

Please Note: the new tab is titled with the name of the new grid you provided and this new tab will appear in the list of active tabs at the top of the grid view.

Conceptual Model 1 X 3D Viewer - 1 X Numerical Grid-Run X Numerical Grid_2 - Numerical Model X

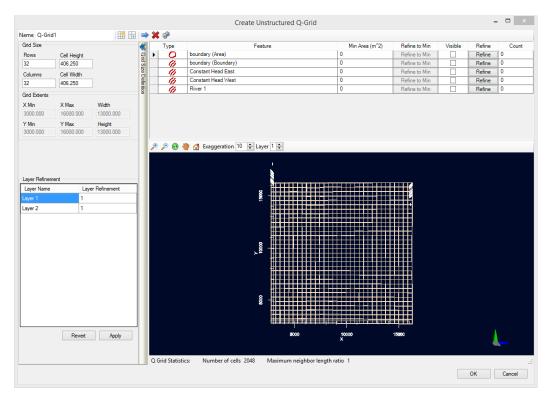
- In addition, this new model run will appear in the model tree. The model run has a grid and corresponding inputs; this can also be seen in the figure above.
- When the conversion is complete, click [[[Next Step) to proceed to the Properties step.

- Now, as explained previously, you can review the properties and boundary conditions, and translate and run this model.
- Once the heads are generated, you can compare this to the results from previous grids.

Using Unstructured Grids

It's also very easy to generate different grid types (such as unstructured V-grids, or quadtree grids (Q-grids) when you use the conceptual modeling workflow. To test these alternate grid types return to the conceptual modeling workflow. On the 'Select Grid Type' workflow step you can select either the 'Define Unstructured V-Grid' or 'Define Unstructured Q-grid' option (the steps below are for a Q-grid example).

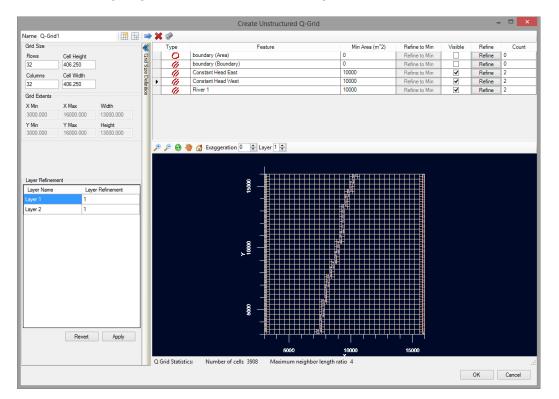
- At the top of the grid view you will see a list of active tabs:
- Click on the first tab, which should be your Conceptual Model workflow ('Conceptual Model 1') to make this the active window, and it should now appear on your display.
- Click [Select Grid Type] from the workflow tree.
- Click [Define Unstructured Q-grid] button and the 'Create Unstructured Q-Grid' window will appear.



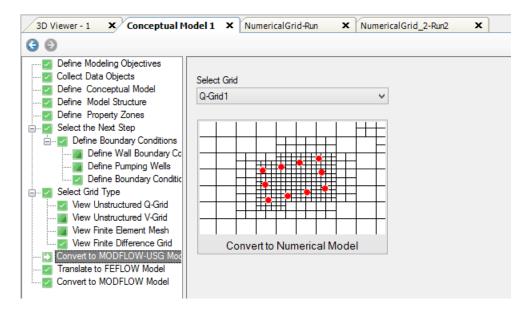
Let's perform a simple refinement around the boundary conditions within the model. Using the table at the top of this window we will visualize the constant head and river boundary condition objects, and refine the cells which contain these boundaries to a desired size.

- Activate the 'Visible' checkbox for the river and constant head (East and West) boundary conditions
- Type '10000' in the 'Min Area (m^2)' field for all three boundary conditions

- Click the 'Refine to Min' button for all three boundary conditions
- The resulting Q-grid should look like the image below:



- Click 'OK' in the 'Create Unstructured Q-Grid' window
- Proceed to the 'Convert to MODFLOW-USG Model' workflow step
- Click on the [Convert to Numerical Model] button to proceed.

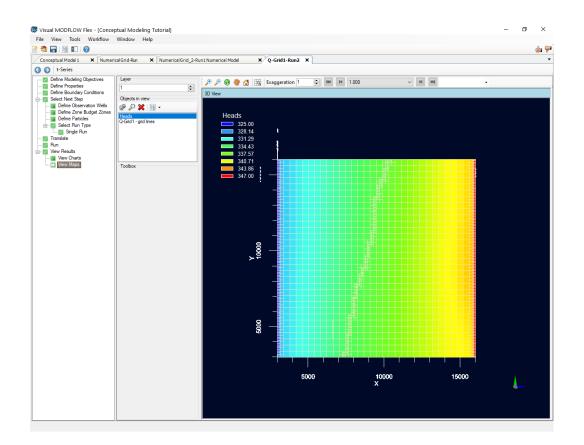


• After clicking on the conversion button, a new workflow window will appear which includes the steps for the numerical model for this new grid. For unstructured grids,

Define Modeling Objectives Define Properties	Flow type	Transport Active				
Define Boundary Conditions	Saturated (Constant Density) \sim	Retardation Model				
Select Next Step Define Observations	Simulation type	No sorption simulated				
Define Zone Budget Zones	Groundwater Flow ~	Reaction				
🖕 Define Particles		No kinetic reactions				
Select Run Type	Available Flow Engines MODFLOW-6					
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	numerical model. This value cannot be changed once it has been set.	Name	Description	Mobile	InitialConcentration (mg/L)	MDCOEF (m ² /day)
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you are able to choose between MODFLOW-USG and MODFLOW-6. For this run, use MODFLOW-6:

- When the conversion is complete, click [(Next Step) to proceed to the Properties step.
- Now, as explained previously, you can review the properties and boundary conditions, and translate and run this model.
- Once the heads are generated, you can compare this to the results from previous grids.
- When the model runs successfully you should see the following results (map of heads in layer 1) for the Q-grid realization of your model:



Compare Model Runs

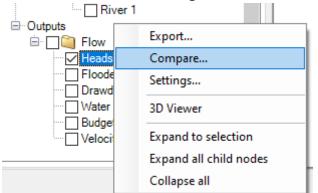
It's possible to run multiple realizations of the same model and compare their model outputs. This is a useful tool for visualizing how changes to things like solver settings, flow engines, and discretizations affect model results.

Let's compare how the results of MODFLOW-6 compares to the results of MODFLOW-USG:

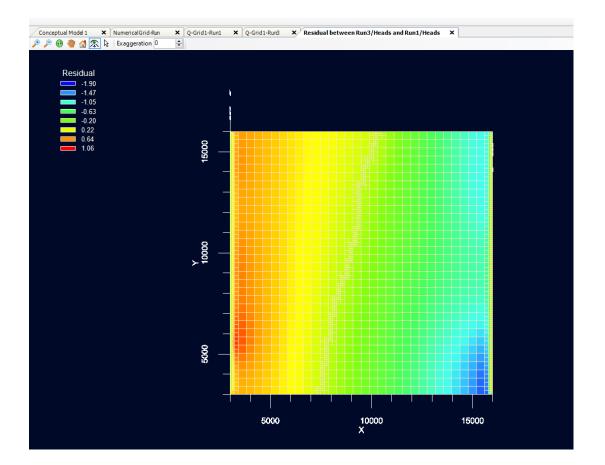
- In the Model Explorer, under Q-Grid, **right-click Run1** (or whatever the run you just finished was named) and **select Clone Model Run...**
- A new workspace tab will open. Always be sure you're working in the correct workspace tab!
- In the new workspace tab, select "Single Run." Select for the flow engine, select "USGS MODFLOW-USG from WH"

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🌌 Define Zone Budget	Zones 📗 🔄 Run Trans	isport Engine	
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- Translate and run the model
- In the Model Explorer, find the Heads outputs that were just calculated, under the Outputs node of the current run. **Right-click** the heads outputs and select **Compare...**



- The Compare Heads dialogue will open. From the Model Explorer, **left-click** to select the Heads outputs from the *original* model run done with MODFLOW-6.
- Select the blue arrow button under "Heads from Numerical Model". The MODFLOW-6 heads should be loaded in. Select **OK** to calculate the residuals between the runs
- You should now see a map of residuals:



As you can see, the conceptual modeling workflow is ideal for generating multiple realizations of your model using different grid types, different levels of grid refinement, etc. This makes scenario analysis easier than ever!

This concludes the Conceptual Modeling tutorial.

3.2 Importing VMOD/MODFLOW Models

The following example is a quick walk-through of the basics of importing an existing Visual MODFLOW Classic or MODFLOW data set.

Objectives

- Learn how to create a project and import an existing numerical model
- Become familiar with navigating the GUI and steps for numerical modeling

- Learn how to view and edit properties and boundary conditions, in a variety of views
- Translate the model inputs into MODFLOW packages and run the MODFLOW engines
- Understand the results by interpreting heads and drawdown in several views
- Check the quality of the model by comparing observed heads to calculated heads

Required Files

This tutorial is designed to allow you to work with the provided example files or you can select your own Visual MODFLOW Classic or MODFLOW project, and follow through the steps. If you wish to use the model that is shown in the following example, it can be found in the Visual MODFLOW Flex documents folder, which is typically:

C:\Users\Public\Documents\Visual MODFLOW Flex\Tutorials\VMOD Import\vmodmodel-import\vmod-model

If you cannot locate these files, they are also available to be <u>downloaded from our website</u>.

Importing a Visual MODFLOW Classic Project

The release of Visual MODFLOW Flex v5.0 introduced a new method of importing Visual MODFLOW Classic projects. This new method simplifies the process to import an existing Visual MODFLOW Classic project. The new method combines the 'Create a new project' and 'import model files' processes into a single step. This section describes the new procedure for importing Visual MODLFOW Classic projects. The old/customary method of importing Visual MODFLOW Classic and other MODFLOW projects is covered in the next section (Create the Project and Import Model Files).

If you import your Visual MODFLOW Classic project using this new method, please follow the steps in this section and then skip ahead to the 'View/Edit Grid' section. Please note that this method does not work for other MODFLOW projects, it is specific to the import of Visual MODFLOW Classic projects.

- Launch Visual MODFLOW Flex S
- Select [File] then [Import Project..].
- Browse to the location of your Visual MODFLOW Classic project and select the Visual MODFLOW Classic file (i.e. wellhead-capture-zone.VMF file). This project file will be contained in the folder:

C:\Users\Public\Documents\Visual MODFLOW Flex\Tutorials\VMOD Import\vmodmodel

- Click [Open].
- The 'Import Visual MODFLOW Classic Project' window will open:

Import Visual Modflow Classic Project	—		\times
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Documents\Visual MODFLOW Flex\Tutorials\VMOD Import\vmod-model\wellhea	ad-capture	-zone.vmf	
Project Name: *			
VMOD Import Tutorial			
Data Repository: *			
C:\Users\msmith\Documents\Visual MODFLOW Flex\Projects			
Create a folder for the project			
Description:			
Import	Cancel	Hel	p

- Enter a project name for the Visual MODFLOW Flex project (by default it will enter the same project name as the Visual MODFLOW Classic project). In this example the project has been named 'VMOD Import Tutorial'
- Select a data repository for the Visual MODFLOW Flex project, select whether to create a folder for the project, and provide a description as required.
- Click [Import]
- A dialogue window will load showing the progress of the model import:

Import Visual Modflow Classic Project	_		\times
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	Close	Help	

The dialogue window should indicate that all model elements have been imported successfully. Note that there may be some warning messages that are generated indicating that there are no distributed concentrations. Dismiss the warning. The following model components will be loaded: grid, model properties, boundary conditions, MODPATH/ZoneBudget inputs (i.e. zones, particles) and observation data.

- Click [Close]
- The new numerical model should be fully loaded, and the 'Define Modeling Objectives' workflow step will be active:

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You can now continue with the regular numerical modeling workflow by proceeding to the section of this tutorial titled View/Edit Grid.

Creating the Project and Import Model Files

This section describes the procedure for importing MODFLOW project files (developed independently of the Visual MODFLOW Classic/Flex interface) into the Visual MODFLOW Flex interface. This procedure can also be used to import Visual MODFLOW Classic projects, but the procedure outlined in the previous section (for Visual MODFLOW Classic projects) is more streamlined.

Launch Visual MODFLOW Flex



- Select [File] then [New Project..]. The Create Project dialog will appear.
- Type in the project name 'Import Tutorial'.

- Click the [^[]] button, and navigate to a folder where you wish your projects to be saved, and click [OK].
- Define your coordinate system and datum (or just leave the local Cartesian as defaults).
- For this project, the default units will be fine.

The Create Project dialog should now look like this (units may be different):

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		Groundwater Flow	m^3/d		
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Description:		Mass	kg		
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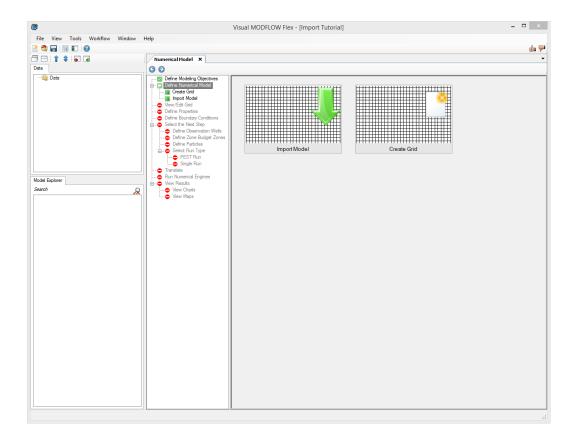
- Click [OK]. The workflow selection screen will appear.
- Select [Numerical Modeling] and the Numerical Modeling workflow will load.
- In this step, you define the objectives of your model and the default parameters.

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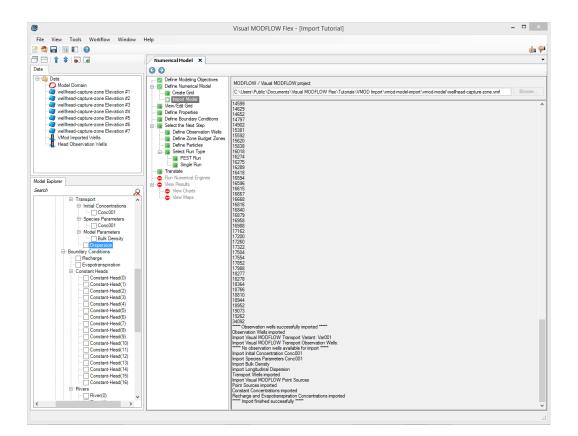
• For the Start Date, expand the date picker, and select 1/1/2000

Please Note: the start date for the numerical model is only relevant should you decide to import pumping well or observation data in absolute times; MODFLOW always uses relative time, with a start time = 0 (days or seconds)

- Click [] (Next Step) to proceed.
- At this step, you can choose to create a new empty numerical grid, or import an existing project.



- Click the [Import Model] button.
- Navigate to the folder that contains your Visual MODFLOW or MODFLOW project. Or you can open the project located in: C:\Users\Public\Documents\Visual MODFLOW Flex\Tutorials\VMOD Import
- Select the file (.VMF [VMOD Classic] or .NAM [MODFLOW] file) and click [Open] to continue. The import will start and you will see the status in the progress window.
 - For VMOD Classic projects, it is usually easier to follow the steps listed in the section above (i.e. simply click File > Import Project... from the main menu, and browse to and select a VMOD Classic project file (.VMF))
 - If the project was built in a different groundwater modeling program than the model name file (.NAM) must be selected instead
- During the import, there are a few things to observe:
- Flex runs a series of validation checks on the MODFLOW projects you import and will display warnings for any anomalies it finds. In the example project provided for this tutorial, Flex will warn you that the wellheads-capture-zone.mbu file is missing from the project you are importing.
- Hit [OK] to continue.



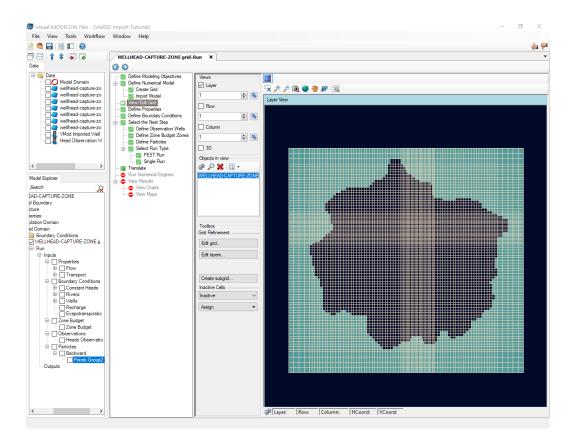
- The status of each model element import is shown in the main window; any detected errors will be shown here.
- After the import, you will see the 'Model Explorer' is populated in the bottom left corner of the screen; from here, you can show/hide different model inputs/outputs.

Please Note: You can add other data objects to the model, such as an image or other raw data (polyline/polygon shapefiles). These files need to first be imported, then they can be displayed at the one of the subsequent steps ('View Grid', 'Define Properties', 'Define Boundary Conditions') or in a 3D viewer by selecting [Window] then [New 3D Window], then checking on the box beside the appropriate data object.

• Click [] (Next Step) to proceed, where you will arrive at the View/Edit Grid step.

View/Edit Grid

- At this step, you can view the numerical grid in layer (plan) view, cross-sectional (along row or column), and 3D view.
- There are numerous tools available to control and manipulate the grid views:



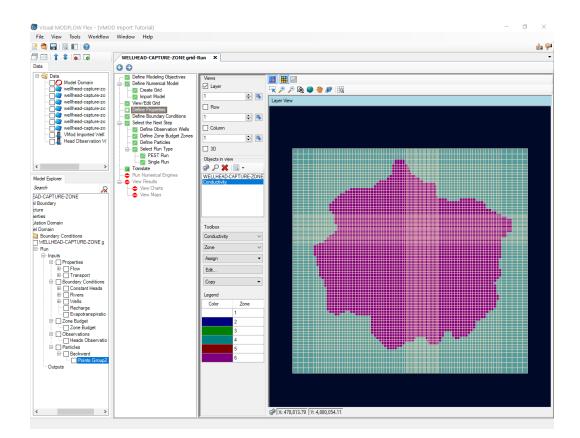
- Under 'Views', select the various views you want to see in the Flex viewer; VMOD Flex allows you to simultaneously show a layer, row, column and 3D Views. Place a check box beside the desired view and it will appear on the screen.
- Adjust a specific layer, row, or column using the up/down arrows. Alternatively, click

on the [>>] button then click on any specific row, column, or layer in any of the 2D views, and the selected row, column, or layer will be set automatically.

- The standard navigation tools allow you to zoom, pan, and in the case of 3D view, rotate.
- Click [[(Next Step) to proceed to the Properties step.

Define Properties

• At the this step, you can view/edit the flow properties for the model, including hydraulic conductivity, storage parameters, and porosity. If you are simulating transport, then transport related properties such as bulk density, dispersion coefficients, sorption, and reaction parameters can also be viewed and edited at this step.



- Under the Toolbox, use the combo box to select from the various Property Groups: Conductivity, Storage, and Initial Heads.
- For each parameter group, you can choose to render by Zones or by a selected attribute. Based on your selection, the color rendering in the views will change.
- Click [Edit...] button to see the conductivity zones that exist in your model and the values in each individual cell.
- Use the same tools as described in the previous step to manipulate the views.
- The display tools will allow you to switch from discrete cells rendering to color shading/contours.

The display tools will allow you to switch from discrete cells rendering to color shading/contours (note, this is available only when you are rendering by an attribute and not when you are rendering by ZoneID)

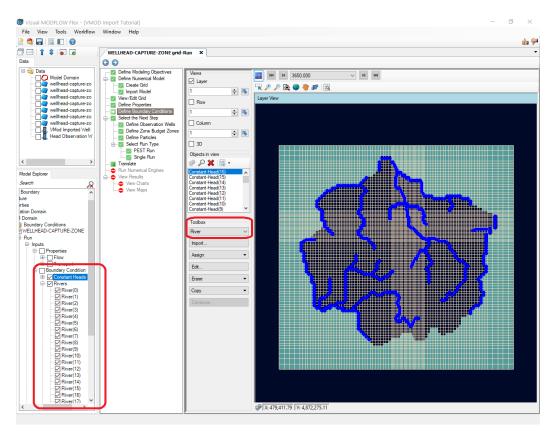
2

Show/hide grid lines Show as cells Show as Surface

- At the bottom of the display, you will see in the status bar the position of your mouse cursor in the current view (XY) grid position (Layer, Row, Column), grid dimension (cell width, length, and thickness), and the Zone ID or attribute value for the selected cell.
- Click [] (Next Step) to proceed to the Boundary Conditions step.

Define Boundary Conditions

 At this step, you can view/edit the flow (and transport) boundary conditions for the model. By default, Constant Heads (if any) will be displayed in the model. In order to see other boundary conditions, you can set these to visible from the Model Explorer (check on the appropriate cell groups or boundary condition category). All cells in a visible (checked) boundary condition will be displayed in a 3D view; however, you will only see in boundary condition cells in the current layer, row, or column in the layer, row, or column views respectively. Also, when you choose another boundary condition from the Toolbox (e.g. River), then this set of boundary condition cells will become visible.

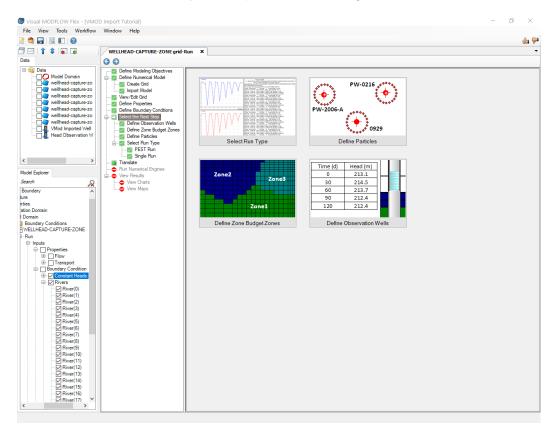


- From the toolbox, select the desired boundary condition group (Constant Head, Rivers, etc..)
- Then select [Edit...].
- Click on a cell that belongs to the boundary you are interested in; a dialog will appear where you can see the parameters for all cells in that boundary. If you want to switch to see values in a different boundary, you can select it in the grid view and the dialog will automatically update to show the new boundary.
- For Recharge or Evapotranspiration, you need to select this Boundary Condition type from the list under the Toolbox, and the Recharge/EVT zonation will appear. A [Database] button will be enabled allowing you to view the zonation.
- You can also assign new boundary conditions to the model using the [Assign] options; for more details, please see <u>Define Boundary Conditions</u>

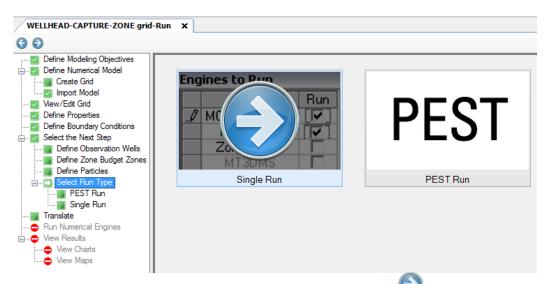
• Click [] (Next Step) to proceed. You will arrive at the "Select the Next Step" options screen

Proceed to Run or Define Optional Model Elements

 You will arrive at a choice screen; where you can proceed to define some of the "nonessential" inputs for the model, such as <u>Zone Budget Zones</u>, <u>Particles</u>, and <u>Observation Wells</u>. Or, you can proceed to setting up a model simulation run.



Click the [Select Run Type] button to proceed (Mouse over this and you will see the blue [] arrow appear on top; just left click once to select this option. (Alternatively, the [] (Next step) button will take you to this step, as it is pre-defined as the default step.)



• Click the **[Single Run button]** to proceed. (Alternatively, the **[Single Run button**] to proceed. (Alternatively, the **[Single Run button**] will take you to this step, as it is pre-defined as the default step.)

Import Model Import Model View/Edit Grid Define Properties Define Boundary Conditions Select the Next Step Define Observation Wells Define Zone Burdget Zones	MODFLOW 2005 from WH Transport Engine IS V IEBUDGET cle Tracking
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- You will arrive at the 'Select Engines' step. Here you can choose which engine(s) you want to run (i.e. what version of MODFLOW-2000, -2005, etc.., and if you want to include MODPATH and ZoneBudget in the run.
- The version of MODFLOW that you used in the Visual MODFLOW Classic model should be selected by default; if you wish to run MODPATH and ZoneBudget, be sure to select these engines as well.

Please Note: ***De-select MT3DMS engine.*** since transport inputs are not fully

defined for this model.

• Click [] (Next Step) to proceed.

Translate Packages

- You will arrive at the 'Translation Step'.
- At this step, you can choose:
 - o whether to run the simulation as steady-state or transient,
 - o the numerical solver you want to use, and
 - o define other MODFLOW package/run settings, such as cell-rewetting, etc.

Some of the translation settings are not fully imported from the Classic model, including the option to run the model as Steady-State vs. Transient (although all of the schedule will be preserved) and the solver settings. These will need to be reviewed and set.For more details, see <u>MODFLOW Translation Settings</u>.

- Click the MODFLOW-2005 > Settings node in the translation tree and verify the following settings:
 - Property Package = BCF6
 - Run Type = Transient

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- Click the MODFLOW-2005 > Solvers node in the translation tree and verify the following settings:
 - Selected Solver = BiCGSTAB-P Matrix Solver (WHS)
 - Max. inner iterations (ITER1) = 50
 - Residual criterion (RCLOSE) = 0.001

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• Click the [Translate] button to proceed; this will read the input from the numerical model and "translate" this into the various input files needed by MODFLOW and the other engines. The files will be created in a file directory in the project structure that is

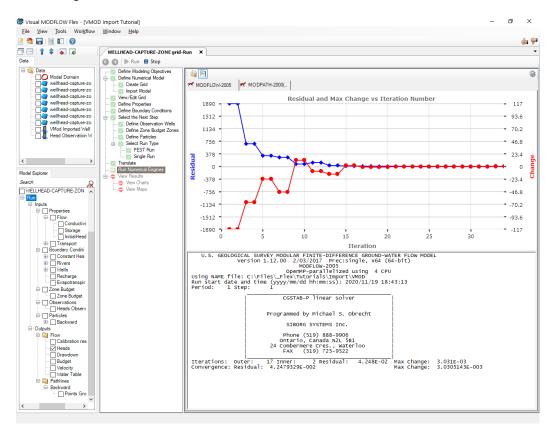
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Click the [] (Next step) button to proceed. You will arrive at the "Run Engines Step".

Run Engines

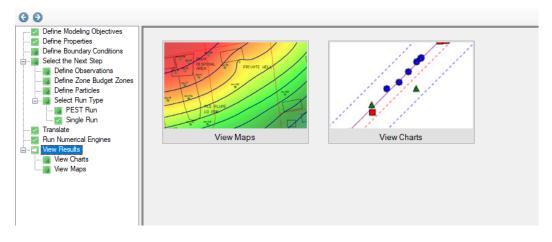
 Click the [Run] button on the main workflow toolbar to start running the engines. You will see a tab for each Engine that includes feedback on the progress of the simulation. Flow and transport engine windows also include a chart of the mass balance residuals and maximum cell value changes as reported by the engine solver. Engine runs that complete successfully with include a green checkmark to the left of the engine tab label.



- Note that after a successful run, the Heads, Pathlines and other output items will be added to the tree in the model explorer.
- Once finished, Click the [[(Next step) button to proceed.

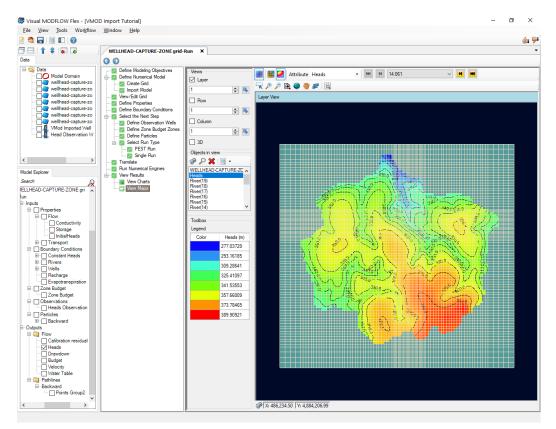
View Results

• You can then choose to view results in the form of Maps (Contours and Color shading) or Charts.



View Maps

- Click the [View Maps] button.
- You will then see color shading of the calculated heads, in layer view.

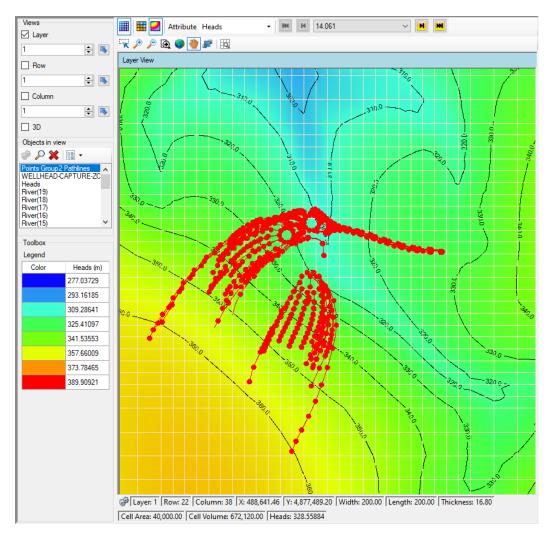


- You can display heads along a row, and along a column, and in 3D, using the same tools as you used earlier. (refer to <u>View/Edit Grid</u> section)
- When the model is transient, you can use the time controls above the Flex Viewer to change the output time; as you do this, all active viewers (layer, row, column, 3D), will refresh to show the heads (or other visible outputs) for the new time.



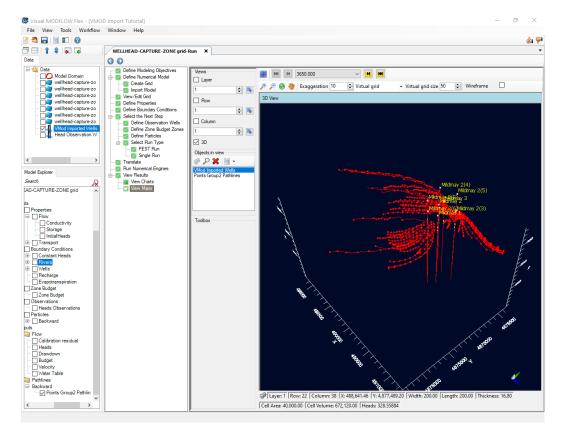
If you ran MODPATH, you will see Pathlines appear as a new node in the 'Model Explorer' tree under Output; add a check box beside the Backward Pathlines (i.e. [Points Group1 Pathlines]) to display these in the active 2D/3D Viewers. You may need to zoom into the middle of the layer view to see the pathlines. (You can automatically zoom to an object by right-clicking on it in the Model Explorer and selecting "Zoom to Object"

Please Note: If you're using the included project and you do not see pathlines, you may need to revise the particle settings before running MODPATH. Right-click the existing particle group object in the Model Explorer and select 'Edit' to change particle group settings. Remember that backward particles should have a release time at the end of the simulation and an end time at the beginning of the simulation.



The pathlines are well represented in a 3D Viewer.

- Turn on the check box beside 3D View, in the available views
- Turn off the check box beside Layer View
- From the Model Explorer, turn off the check box beside Heads
- From the Data explorer (raw data), turn on the check box beside "Vmod Imported Wells"
- Take a moment to rotate your 3D view, and zoom in, and you can get a display similar to the one shown below.



You can also display velocity vectors, which will allow you to easily display and interpret flow fields.

- Turn off the check box beside 'Points Group 1 Pathlines' in the Model Explorer
- Turn on the 'Velocity' output option, in the Model Explorer under 'Outputs' > 'Flow'
- Access the Velocity display settings by right-clicking and selecting 'Settings'
- In the Settings window, access the 'Style' > 'VelocityMap' settings

Velocity vectors may be displayed using average linear or Darcy velocities. In-plane velocity vectors can be displayed using the full magnitude of the vector (i.e. the out-of-plane velocity component will be included), as a projection (i.e. only the in-plane velocity component is displayed), or simply a directional indicator (i.e. the size of the arrow is not dependent on the actual velocity). By default, the velocity vectors will initially be displayed as a projection with average linear velocity values, on a linear scale.

A normal velocity color map function is also supported, which allows you to interpret flows perpendicular to the selected layer/row/column (i.e. out-of-plane flow). By default the normal

velocity color map will be displayed with a red/blue color scheme, with red areas indicating flow inward (i.e. corresponding to the positive X, Y or Z direction), and blue areas indicating flow outward (i.e. corresponding to the negative X, Y or Z direction). Areas with velocities below the specified in-plane range threshold will be displayed using the specified In-plane color (which is grey by default). You can find more information about the velocity map display settings in the <u>3D Gridded Data</u> section of this manual.

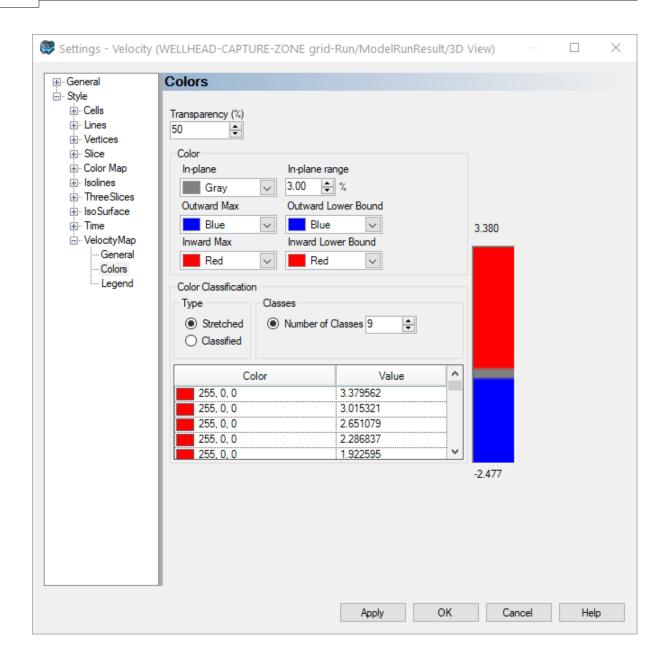
Update the velocity map settings as follows:

- In the 'Color' frame, select the 'Custom' option, and select 'Yellow' as the display color
- In the 'Velocity type' frame, select the 'Darcy' option
- In the 'Scale factor' frame, type a scale factor of 3.0
- Deselect the 'Show legend' option, so that the legend will be hidden

The Velocity should be similar to the following:

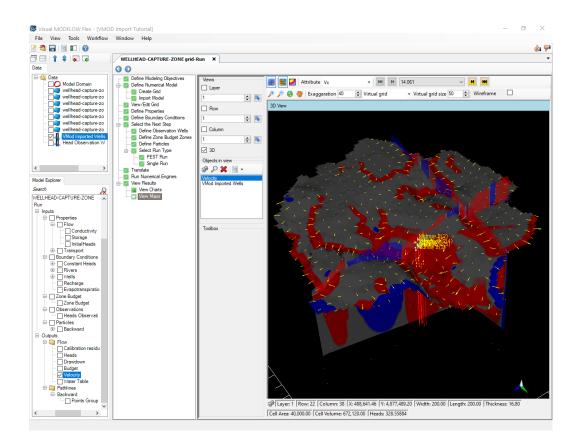
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- Click Apply
- Select the Colors tab and set the In-plane range to 3.00%



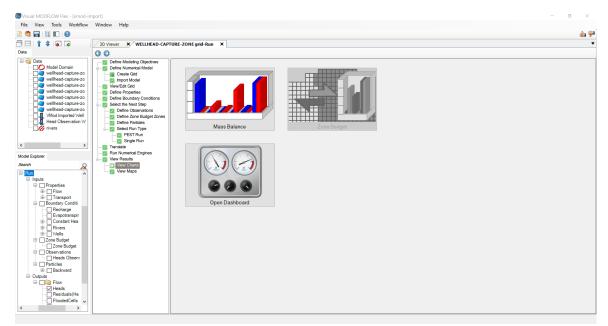
Click OK

Take a moment to rotate your 3D view, and zoom in, and you can get a display similar to the one shown below.

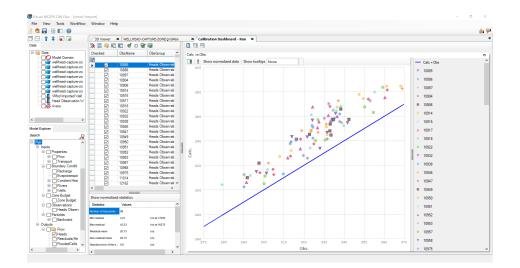


View Charts

- Click 'View Charts' from the workflow tree. You can open the Mass Balance, Zone Budget, or Open Dashboard at this step. For this tutorial, we will click on Open Dashboard.
- Click [Open Dashboard] to proceed.



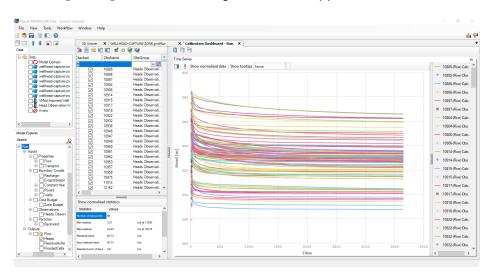
• The following window will appear:



• Take a moment to view the correlation between calculated and observed heads.

Note that the values of the calculated heads are all greater than their respective observed values. This indicates that the model may require some adjustments to more accurately fit the observations. As an optional challenge, see if you can improve the fit.

- Click 'Chart selector' [
- Then, under 'Chart selector' select 'Time Series' and deselect "Calc vs. Obs"
- Click [Close] and the following window will appear:



In the chart above, there are many time series data - the chart may be more easy to interpret if you look at one (or a small) number of charts at a time. You can use the filtering tools in the first row of the tabulated data to filter the data shown on the chart.

*****This concludes the 'Importing Visual MODFLOW/MODFLOW Models' tutorial.*****

3.3 Airport Numerical Model with Transport

The following example walks through creating a numerical model with groundwater flow (using MODFLOW-2005) and basic contaminant transport (using MT3DMS). The exercise is based on the well-known Airport example from Visual MODFLOW Classic.

Objectives

- Learn how to create a project and create a numerical grid
- Become familiar with navigating the GUI and steps for numerical modeling
- · Learn how to define new property zones and boundary conditions
- Define inputs for contaminant transport
- Translate the model inputs into MODFLOW and MT3DMS packages
- Run MODFLOW-2005 and MT3DMS engines
- Understand the results by interpreting heads, drawdown, and concentrations in several views
- Check the quality of the model by comparing observed heads to calculated heads, and observed vs. calculated concentrations

Please Note: if you are unable to locate some supporting files for the tutorial, you may download these from the website.

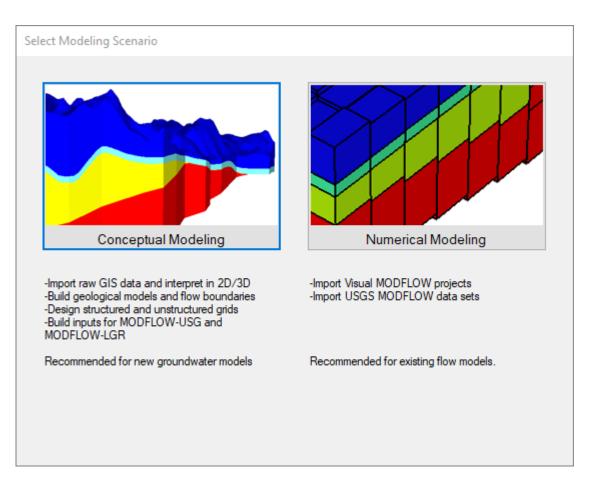
Create the Project

- Launch Visual MODFLOW Flex.
- Select [File] then [New Project..]. The Create Project dialog will appear.
- Type in project name 'Airport Tutorial'.
- Click the [¹] button, and navigate to a folder where you wish your projects to be saved, and click [OK].
- Define your coordinate system and datum (or just leave the Local Cartesian as defaults).

For this project, the default units will be fine. The Create Project dialog should look similar to the following:

Create Project				?	×
Project Information	Uni	ts *			
Name: *		2↓			
Airport Tutorial	~	Unit Settings			
		Concentration	mg/L		
Data Repository: *		Conductivity	m/s		
C:\Users\Public\Documents\Visual MODFLOW Flex\1		Density (includes Bulk	De kg/m^3		
		Groundwater Flow	m^3/d		
Create a folder for the project		Length	m		
Description:		Mass	kg		
Description:		Mass Flow	mg/yr		
		Pumping Rate	m^3/d		
		Recharge	mm/yr		
		Specific Storage	1/m		
		Stream Flow	m^3/d		
		Temperature	°C		
		Time	day		
Project Coordinate		Volumetric Flow	m^3/d		
Coordinate Systems: *					
Local Cartesian 🗸					
Datum: *	Co	oncentration			
World Geodetic System 1984					
		OK	Cancel	H	lelp

• Click **[OK]**. The workflow selection screen will appear.



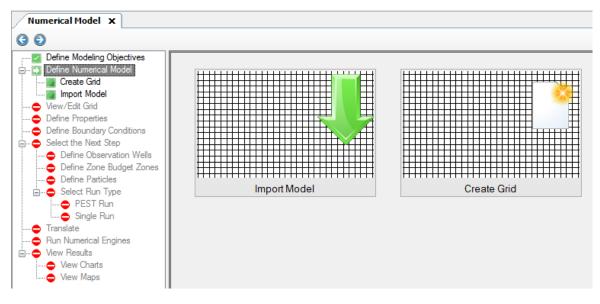
- Select [Numerical Modeling] and the Numerical Modeling workflow will load.
- The first step is to Define Modeling Objectives.

Define Modeling Objectives

- In this step, you define the objectives of your model and the default parameters.
- The **Start Date** of the model corresponds to the beginning of the simulation time period.
- Select 1/1/2000 for the Start Date
- For this scenario, we will include contaminant transport in the model run. **Click the check box beside 'Transport Active'** (in the right hand side of the window, under Define Modeling Objectives.
- For 'Retardation Model' select 'Linear isotherm (equilibrium-controlled)'. For this tutorial you will not be simulating any decay or degradation of the contaminant, so the default 'Reaction' setting of 'No kinetic reactions' will be fine.
- Below the 'Retardation Model' and 'Reaction' settings are two tabs: 'Species Parameters' and 'Model Parameters'. By default, one species (chemical component) is defined for the transport run. For this example, we will leave the initial concentration ('InitialConcentration (mg/L)') as zero, but adjust Kd (the distribution coefficient)
- Type 1E-7 in [Kd 1/(mg/L)] column

😻 Visual MODFLOW Flex - [Airport Tutorial]								- 0	×
<u>File View Tools Workflow W</u> indow	Help								
2 4 🕞 💀 🗉 🕖									💩 🗭
	Numerical Model ×								-
Data	6 0								
Data Data Data Node Ecolorer Saarch	Control Manual Control Co	For type Saturated Constart Density) Saturated Constart Density) Simulation tope Consultater Flow Available Flow Engines USSS MORE/ICVW 2000 html WH MORE/ICVW 2000 html WH	Transpot Active Retardation Model Linear is otherm (equal Reaction No kinet reactions Nobel Cover Service Nobel Cover Service Species Parametere Nobel Cover Service Name Concoort Datebulion coefficient	Nodel Parameters Description Concolor1	Moble 2	Held/Concentration (mp/L) 0	MCCOEF (m ⁻² /dsy) 0	Kd (1/img/L) 1e-7	

- You are now finished setting up the flow and transport objectives. Click [] (Next Step) to proceed.
- The following **'Define Numerical Model'** step will appear; at this step, you can import Visual MODFLOW Classic or MODFLOW data sets, or define a new empty grid. For this tutorial we will create a new grid.



• Click on [Create Grid] to proceed

Create Grid

- At this step, you can specify the dimensions of the Model Domain, and define the number of rows, columns, and layers for the finite difference grid. **Type** the following into the Grid Size section,
- Columns: 40

- Rows: 40
- For Grid Extents, enter 2000 for Xmax and 2000 for Ymax
- Under Define Vertical Grid, Type 3 for Number of Layers

Define Layer Elevations

- In Visual MODFLOW Flex, you can define the elevations of the tops and bottom of the model layers. Or you can have varying layer elevations defined from Surface data objects. Surfaces could be from data objects you imported from Surfer (.GRD, ESRI .ASI, .DEM), or from Surfaces you have created through interpolating XYZ points. In this exercise, you will import 4 surfaces (from Surfer .GRD files), then use these to define the layer elevations.
- Click [File] then [Import Data...] from the main menu. The following window will appear:

************************************	Data Import	- 🗆 🗙
Data Source		
Data Type: * Point		¥
		•
Source File: *		
Name: *		
Name.		
Description:		
	< <back next="">> Cancel Help</back>	1
		1

- For the Data Type, select 'Surface' from the drop-down list.
- In the Source File field click the [...] button and navigate to your Public "My Documents" folder, then "Visual MODFLOW Flex\Tutorials\Airport\suppfiles\Surfer\airport-ground-surface.grd" and select [Open]
- Click [Next>>]
- Click [Next>>] (accept the defaults)
- Click [Next>>] (accept the defaults)
- Click **[Finish]**. You should now see a new "airport-ground-surface" data object appear in the data tree, in the top left corner of the window.
- Now, repeat the above steps to import the other Surfer .GRD files into the project:

- o airport-layer2-top.grd
- o airport-layer3-top.grd
- o airport-layer3-bottom.grd
- When you are finished, you should see 4 Surface data objects in the data tree in the top left corner.
 - Data
 Data
 Data
 airport-ground-surface
 airport-layer2-top
 airport-layer3-top
 airport-layer3-bottom
- Now you are ready to define the grid layers using these surfaces. Under Number of Layers, **select 'Use Surface' check box** for <u>each</u> grid layer. This is shown below

Number of Layers				
Layer Name	Use Surface	Surfaces	Elevation	
Layer 1 - Top	•		100	-
Layer 2 - Top	✓		66.666666666667	-
Layer 3 - Top	•		33.33333333333333	-
Layer 3 - Bottom	~		0	

- Next you will provide a surface for each layer;
- Click on airport-ground-surface from the data object tree (it should become

selected), then click on the topmost blue arrow [beside 'Use Surface' in the Number of Layers table (in the row that starts "Layer 1 - Top". If you have done this correctly, the table should appear as shown below.

Number of Layers				
Layer Name	Use Surface	Surfaces	Elevation	
Layer 1 - Top	~	airport-grou	21.20 ~ 16.52	-
Layer 2 - Top	~		66.66666666666	-
Layer 3 - Top	~		33.33333333333333	-
Layer 3 - Bottom	~		0	-

- Now repeat these steps for the remaining layers:
- Select airport-layer2-top Surface data object to the tree, and insert this (using the [

]) as the Surface for Layer 2 - Top

- Select airport-layer3-top Surface data object to the tree, and insert this (using the [
]) as the Surface for Layer 3 Top
- Select **airport-layer3-bottom** Surface data object to the tree, and insert this (using the

]) as the Surface for Layer 3 - Bottom

• When you are finished, the table should appear as shown below.

Number of Layers 3 🔶				
Layer Name	Use Surface	Surfaces	Elevation	
Layer 1 - Top	-	airport-grou	21.20 ~ 16.52	4
Layer 2 - Top	~	airport-layer	13.44 ~ 10.37	4
Layer 3 - Top	~	airport-layer	10.17 ~ 4.55	4
Layer 3 - Bottom	~	airport-layer	2.02 ~ -1.86	

- You are finished defining the layer elevations.
- Click on the **[Create Grid]** button (near the top right of the window) to create the grid. You will see the model tree will be generated on the left side of the window, and **'NumericGrid1'** should appear as the last item.

Refine the Grid

This section describes the steps necessary to refine the model grid in areas of interest, such as around the water supply wells, refueling area, and area of discontinuous aquitard. The reason for refining the grid is to get more detailed simulation results in areas of interest, or in zones where you anticipate steep hydraulic gradients. For example, if drawdown is occurring around the well, the water table will have a smoother surface if you use a finer grid spacing. Also, layer properties can be assigned more correctly on a finer grid.

- Right click on the 'NumericalGrid1' from the tree, and select [Edit Numerical Grid...]
- The following window will appear:

	Edit grid –	
arid edit details Script		
New grid name		
NumericGrid1_refined	Layer 1 😑 🔎 🔎 🌘 🍓	
Overwrite existing grid		
Edit rows		
C Edit columns		
From 10		
To 30		
Replace every		
1 ♥ row{s} with		
2		
Refine rows 1:2		
Apply grid edit Undo edit Reset		
Quality indicators		
Max ratio threshold		
1.50 🖨 😹		
 Highlight cells exceeding threshold 		
Minimum cell size (m) Maximum cell size (m)		
Width Width 50 50		
Height Height		
50 50	Row: 2 Column: 35 X: 1496.13 Y: 2058.25 Cell width: 50 Cell height: 50	
	Add objects using the Data and Model Explorer tree checkboxes	
	OK Cancel	Help
	UK Cancel	нер

The grid refinement works by defining a starting row number, and ending row number, then a 'Refine by' factor; to help you define the limits of where the refinement should be applied, you can add data objects to this display, such as well locations, arial maps, shapefiles, etc. When you are using this feature with your own models, you will need to import these data object files before starting the 'Grid Refinement' step.

- You will first start by refining the rows.
- Enter '5' in the 'From' field, and enter '35' in the 'To' field.
- Enter 'Replace Every [1] row(s) with [2]'. Your screen should appear as follows:

	Edit grid –	
Grid edit details Script		
New grid name		
NumericGrid1_refined	Layer 1	
Overwrite existing grid		
Edit rows		
O Edit columns		
From 5		
To 35		
Replace every		
row{s} with		
2		
Refine rows 1:2		
Apply grid edit Undo edit Reset		
Quality indicators		
Max ratio threshold		
1.50 🚖 📷		
 Highlight cells exceeding threshold 		
Minimum cell size (m) Maximum cell size (m)		
Width Width		
50 50		
Height Height	Row: 6 Column: 1 X: -341.75 Y: 1427.70 Cell width: 50 Cell height: 50	
55	Add objects using the Data and Model Explorer tree checkboxes	
	OK Cancel	Help

- Click on the [Apply grid edit] button.
- Next, you will refine the columns.
- At the top left of the window, select the [Edit Columns] radio button.
- As before, Enter '5' in the 'From' field, and enter '35' in the 'To' field.
- Enter Replace every [1] column(s) with [2]
- Click on the [Apply grid edit] button.

You should now see coarse grid sizes around the edge of the model domain, and a more finer sized grid spacing in the middle of model (around the areas interest). This is shown below. The band of pink cells around the edges of the refinement indicate cells where the Max ratio threshold quality indicator (which is set by default to a cell step size of 1.50) has been exceeded. This can sometimes result in larger computational times and the potential for increased grid based dispersion. These areas can be further fractionally refined to improve the grid quality; in this exercise, we will leave the grid as-is and proceed to the next step.

	Edit grid	- 🗆 🛛
Grid edit details Script		
New grid name		
NumericGrid1_refined	Layer 1	
Overwrite existing grid		
O Edit rows		
Edit columns		
From 17		
To 53		
Replace every		
column(s) with		
2		
Refine columns 1:2		
Apply grid edit Undo edit Reset		
Quality indicators		
Max ratio threshold		
1.50 🚖 📷		
 Highlight cells exceeding threshold 		
Minimum cell size (m) Maximum cell size (m)		
Width Width		
25 50 Height Height		
25 50	Row: 1 Column: 24 X: -351.53 Y: 1975.15 Cell width: 50 Cell height: 50	
55	Add objects using the Data and Model Explorer tree checkboxes	
	OK Cancel	Help

• Click on the [OK] button.

In the Model Explorer tree, a new grid and numeric workflow (i.e. 'NumericGrid1_refined') is created, and a new workflow window/tab (i.e. 'NumericGrid1_refined-Run1') opens. At this stage we will continue working with the refined grid, and we can ignore the initial coarse grid.

- In the next section, you will view the numerical grid that you just created.
- Click on the Define Properties step or click the next button [] to proceed.

Define Flow Properties

This section will guide you through the steps necessary to design a model with layers of highly contrasting hydraulic conductivities.

- First, ensure that **'Conductivity'** is selected in the first dropdown menu under the **'Toolbox'**
- Click on the **[Edit...]** button and Type the following values in the top row of the window:
 - Kx (m/s): 2E-4, then use [F2] to propagate through all cells
 - Ky (m/s): 2E-4, then use [F2] to propagate through all cells
 - Kz (m/s): 2E-4, then use [F2] to propagate through all cells
- Click **[OK]** to accept these values.

Please Note: it may take a moment for Flex to process this change.

In this case the Kx, Ky, and Kz values are the same, indicating the assigned property values are assumed horizontally and vertically isotropic. However, anisotropic property values can be assigned to a model by modifying the Conductivity Database.

In this three layer model:

- Layer 1 represents the upper aquifer
- Layer 2 represents the aquitard separating the upper and lower aquifers, and
- Layer 3 represents the lower aquifer.

For this example, we will use the previously assigned hydraulic conductivity values (Zone# 1) for model layers 1 and 3 (representing the aquifers) and assign different Conductivity values (i.e. a new Zone) for model layer 2 (representing the aquitard). Note that layer 1 is the top model layer.

• Next you need to change to Layer 2. (using the up arrow under the Layer text box shown below)

Views	
✓ Layer	
2	÷ 🔻
Row	
1	÷ 🔻
Column	
1	÷ 🔻
🗌 3D	

You are now viewing the second model layer, representing the aquitard. The next step in this tutorial is to assign a lower hydraulic conductivity value to the aquitard (layer 2). We can graphically assign the property values to the model grid cells.

• Click [Assign] then [Entire Layer/Row/Column] from the toolbox.

The following dialog will appear:

one	ttributes	New							Select data object (Drag from Data Tree) Image: polygon Holes in polygons will be ignored
	Parameter	Unit	Method		Value		Object	Mapping	 Assign between sulfaces Top sulface:
•	Kx Ky	m/s m/s	Constant Constant		0.0002	→			
	Kz	m/s	Constant	¥	0.0002			~	
									Assign to all layers Layer 1 Layer 2 Layer 3

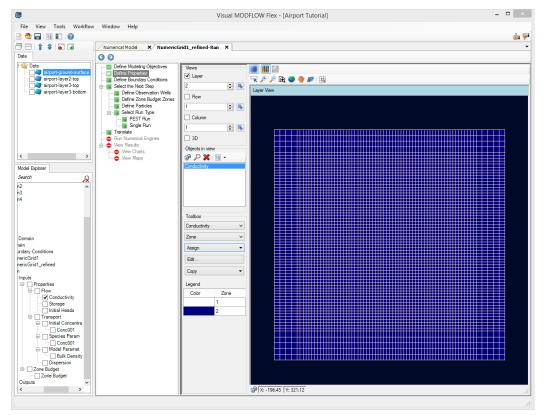
- Click on the **[New]** button at the top; this will create a new zone.
- Enter the following values:
 - Kx (m/s): 1E-10
 - Ky (m/s): 1E-10
 - Kz (m/s): 1E-11

The dialog should appear as shown below:

					New	Proper	ty Zone			
Zone 2 Zone	Attributes	New								t data object (Drag from Data Tree) polygon Holes in polygons will be ignored
	Parameter	Unit	Method		Value		Object	Mapping		ssign between surfaces Top surface:
	Kx	m/s	Constant	~	1E-10			_	-	
	Ку	m/s	Constant	~	1E-10				~	Bottom surface:
▶	Kz	m/s	Constant	¥	1E-11				~	
										Assign to all layers Layer 1 Layer 2 Layer 3
										OK Cancel

• Click [OK] to accept these values.

Once finished, the cells for Layer2 should change blue, which indicates these cells belong to Zone2; you can use the Legend under the toolbox as a guide, and also mouse over cells in the grid view, and note the values in the status bar.



Next you must assign the appropriate conductivity values to the discontinuous region. Although the region where the aquitard pinches out is very thin, the conductivity values of these grid cells should be set equal to the Conductivity values of either the upper or lower aquifers. In this particular example, the zone of discontinuous aquitard is indicated on a shapefile. We will import this shapefile into the project:

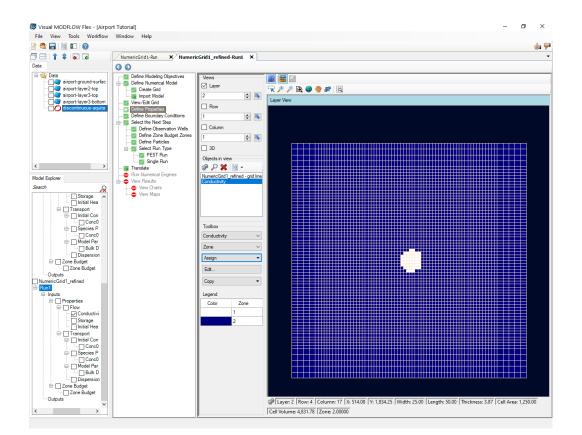
- Click [File] then [Import data...]
- For the Data Type, select Polygon from the drop-down list.
- In the Source File field click the [...] button and navigate to your Public "My Documents" folder, then 'VMODFlex\Tutorials\Airport\suppfiles\discontinuous-aquitard.shp', and click [Open]
- Click [Next>>]
- Click [Next>>] (accept the defaults)
- Click [Next>>] (accept the defaults)
- Click [Finish].
- You should now see a new data object, 'discontinuous-aquitard' appear in the data tree, in the top left corner of the window.
- Click on the box beside this data object in the tree
- The data object should now appear in the Layer View of the grid.
- Zoom into this area (using the mouse wheel, or the Zoom in button on the toolbar).

150

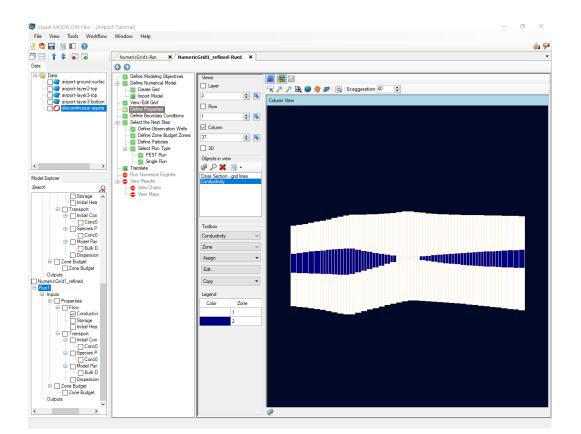
- Click [Assign] then [Using Data Object] from the toolbox.
- Use the [button to pull in the **discontinuous-aquitard** shape file in the new property zone window (you can also drag/drop a data file into this field)
- We want to assign these cells to an existing Zone: Zone1 that represents the aquifer above. So in this case, it is not necessary to create a new parameter zone. Use the zone arrows to select Zone 1 and verify that the K-values are all 0.0002 and that Layer 2 is selected (i.e. the checkbox for layer 2 is checked in the 'Assign to Layers' section). Your screen should look like the following:

Nev	w Property Zone										
Zor	ne							Select data object (Drag from Data Tree)			
1	+	New						discontinuous-aquitard			
Zor	ne Attributes		Holes in polygons will be ignored								
	Parameter	Unit	Method	Value		Object	Mapping	 Assign between surfaces 			
►	Kx	m/s	Constant	0.0002			~	Top surface:			
	Ку	m/s	Constant	0.0002			~	Bottom surface:			
	Kz	m/s	Constant	/ 0.0002	⇒		~				
								Assign to layers			
								Assign to all layers			
							Layer 1				
								Layer 2			
								OK Cancel			

• Click **[OK]** to assign this group of cells to Zone1. This display should appear as shown below.



- Now view the model in cross-section to see the three hydrogeological units. First, zoom out to the fill extent using one of the following options:
 - Zoom out button from the toolbar
 - Zoom full extents button from the toolbar
 - Scroll wheel on the mouse (scroll forwards)
- Click the **[Column]** check box in the 'Views' section. You will see another view appear beside the layer view, showing a cross-section through the model domain (by default, through Column1). To improve this view, you should change the Exaggeration
- Enter 40 in the Exaggeration field, which is located in the toolbar directly above the Column view window.
- Enter 37 for the Column number, as this will provide a cross-section through the region with the discontinuous aquitard. Take a moment to view the cross-section of the properties. You can also change the cross-section view (change the Column number up, down, or enter a new value), and use the zoom and pan tools on the Column view to improve the display. Note that you can repeat the same steps above for Rows, instead of Columns, in order to see cross-sections along the X-axis.
- The display should look similar to the image below:



- When you are finished, turn the Column View off, by **removing the check-box beside** [Column] under 'Views'.
- Now is a good time to save the project. Click [File] then [Save Project] from the main menu.
- Click [[(Next Step) to proceed.

Define Boundary Conditions

The next step is to define the flow boundaries for the model. In this example, you will define:

- constant heads along the north edge of the model domain in layers 1 and 3,
- the Waterloo River along the southern portion of the model in layer 1,
- a constant head along the southern edge of the model in layer 3, and
- two recharge zones with differing rates applied at the top of the model (ground surface)

You will also import and define pumping wells in the next section of this tutorial.

Constant Heads

The first Constant Head boundary condition will be for the upper unconfined aquifer along the northern boundary of the model domain. To do this you will use the **[Assign]>[Polyline]** tool.

- First, you need to go back to Layer 1. Type '1' into the [Layer] field under 'Views' (or use the arrow buttons).
- Next, ensure that 'Constant Head' is selected from the first dropdown menu under the 'Toolbox' section.
- Under the 'Toolbox' section, click [Assign]>[Polyline]. Move the mouse pointer to the north-west corner of the grid (top-left grid cell) and left-click on this location to anchor the starting point of the line. Now move the mouse pointer to the north-east corner of the grid (top-right grid cell) and Right-Click on this location to indicate the end point of the line. Click 'Finish', then you should then see a small menu appear to 'Define Boundary Condition'.
- Click [Next >>] to accept the default name.
- Enter Starting Head (m) of 19 in the top row and hit F2 to propagate this value.
- Enter Ending Head (m) of 19 in the top row and hit F2 to propagate this value.
- Leave the default value of -1 for Conc001; this indicates that no contaminant mass will be assigned to these cells.

chedule Static 🔹 🚟 🧱	Na	ime Con	stant	Head 1		🔒 🙀 Calculation 19	\sqrt{x}) 🏥 🎟 📰 🖋		
This boundary condition is static. Switch to		Layer	V	Row 🛛	Column 🗸	Starting Head (m 😙	Ending Head (m) 🍸	Conc001 (mg/L) 🍸	Active 🛛	
ransient to define a schedule.		1		1	1	19	19	-1	\checkmark	
		1		1	2	19	19	-1	\checkmark	
		1		1	3	19	19	-1	\checkmark	
		1		1	4	19	19	-1	\checkmark	
		1		1	5	19	19	-1	\checkmark	
		1		1	6	19	19	-1	\checkmark	
		1		1	7	19	19	-1	\checkmark	
		1		1	8	19	19	-1		
		1		1	9	19	19	-1	\checkmark	
		1		1	10	19	19	-1	\checkmark	
		1		1	11	19	19	-1		
		1		1	12	19	19	-1		
		1		1	13	19	19	-1		
		1		1	14	19	19	-1		
		1		1	15	19	19	-1		
				1	16	19	19	-1		
		1		1	17	19	19	-1		
				1	18	19	19	-1		
Assign to appropriate layer		1		1	19	19	19	-1		

• Click [Finish] to complete the boundary condition. The hand-drawn polyline will now turn to a set of red points, indicating that a Constant Head boundary condition has been assigned to these cells. The display should look like the image below:

Next you will assign a Constant Head boundary condition along the northern boundary for the lower confined aquifer.

• Locate the [Layer] selection in the 'Views' section, and change this to '3'.

Views	
✓ Layer	
3	÷ 🔻
Row	
1	÷ 🐴
Column	
1	÷
🗌 3D	

- Ensure that 'Constant Head' is still selected from the first menu under the 'Toolbox' section.
- Click [Assign]>[Polyline] from the toolbox. Move the mouse pointer to the north-west corner of the grid (top-left grid cell) and left-click on this location to anchor the starting point of the line. Now move the mouse pointer to the north-east corner of the grid (top-right grid cell) and right-click on this location to indicate the end point of

the line. Click 'Finish' then you should then see a small menu appear 'Define Boundary Condition'.

- Click [Next >>] to accept the default name.
- In the Define Boundary Condition dialog, enter the following values:
- Enter Starting Head (m) of '18' in the top row and hit F2 to propagate this value.
- Enter Ending Head (m) of '18' in the top row and hit F2 to propagate this value.
- Click **[Finish]** to complete the boundary condition. The hand-drawn polyline will now turn to a set of red points, indicating that a Constant Head boundary condition has been assigned to these cells

Next, assign the Constant Head boundary condition to the lower confined aquifer along the southern boundary of the model domain.

- Click [Assign]>[Polyline] from the toolbox. Move the mouse pointer to the south-west corner of the grid (bottom-left grid cell) and click on this location to anchor the starting point of the line. Now move the mouse pointer to the south-east corner of the grid (bottom-right grid cell) and right-click on this location to indicate the end point of the line. Click 'Finish' then you should then see a small menu appear 'Define Boundary Condition'.
- Click [Next >>] to accept the default name.
- In the Define Boundary Condition dialog, enter the following values:
- Enter Starting Head (m) of '16.5' in the top row and hit F2 to propagate this value
- Enter Ending Head (m) of '16.5' in the top row and hit F2 to propagate this value.
- Click **[Finish]** to complete the boundary condition. The hand-drawn polyline will now turn to a set of red points, indicating that a Constant Head boundary condition has been assigned to these cells

River

The following instructions describe how to assign a River boundary condition in the <u>top</u> layer of the model, along the southern edge of the model.

- First, you need to go back to Layer 1. Type '1' into the [Layer] field under 'Views' (or use the arrow buttons).
- Now we need to import our river data object (using the steps explained previously; [File]>[Import Data]>'Polyline'>'river.shp')
- Select 'River' from the first dropdown menu in the 'Toolbox' section.
- Click **[Assign]>[Using Data Object]** from the toolbox. Use the **[**] button to add the river data object to the geometry section of the **'Define Boundary Condition'** dialog. Hit **[OK]** to the message that the extents will be clipped to the model domain.
- Click [Next>>] to accept the default name.
- The 'Define Boundary Condition' window will appear as shown below.

Soundary Condition Script										
Schedule Static 🔹 🗰 🧱	Name	River 1		🛛 🏠 Calc	ulation	🗮 🎟 🗷 🖋 🗐				
This boundary condition is static. Switch to	Layer	Row T	Colum 🖓	River Stage (m) V	Riverbed Bottom (m) V	Conductance (m^2/d	River Width (m) 🛛	Riverbed Thickness (m) V	Riverbed Kz (m/s) 🗸	Acti 🛛
transient to define a schedule.	•	19	53							
		1 20	53							
		1 20	52							
		1 21	52							
		1 21	51							
		1 22	51							
		22	50							
		23	50							
		23	49							
		1 24 1 25	49							
		1 25	49							
		1 25	48 48							N
		1 26	40							
	_	20	47							
		27	46							
	_	27	46							
	_	28	45							
		29	45							N N
Assign to appropriate layer										

Traditionally, the River boundary condition has required a value for the conductance of the riverbed. However, the conductance value for each grid cell depends on the length and width of the river as it passes through each grid cell. Therefore, in a model such as this, with different sizes of grid cells, the conductance value will change depending on the size of the grid cell. In order to accommodate this type of scenario, Visual MODFLOW Flex allows you to enter the actual physical dimensions of the river at the Start point and End point of the line, and then calculates the appropriate conductance value for each grid cell according to the standard formula.

Select the first row in the define Boundary Condition dialog and notice Flex has highlighted in yellow the corresponding river cell (lower left corner of the river). This dialog is interactive; you can select cells in the dialog or viewer/grid window to see how boundary values are currently assigned.

• In the top row of the boundary assignment dialog enter the following values for the start point.

River Stage (m)	16.0
Riverbed Bottom (m)	15.5
Conductance (m^2/day)	(automatically calculated based on width, thickness and Kz)
River Width (m)	25
Riverbed Thickness (m)	0.1
Riverbed Kz (m/s)	1E-4

Leakance from the river will be calculated based on the parameters you define. For more details on the calculation, refer to <u>Boundary Conditions Theory</u>

- Now you will define the values for the End Point of the river.
- Scroll to the bottom row in the Define Boundary Condition dialog and click in it. Notice the river end cell is now highlighted yellow in the grid view.

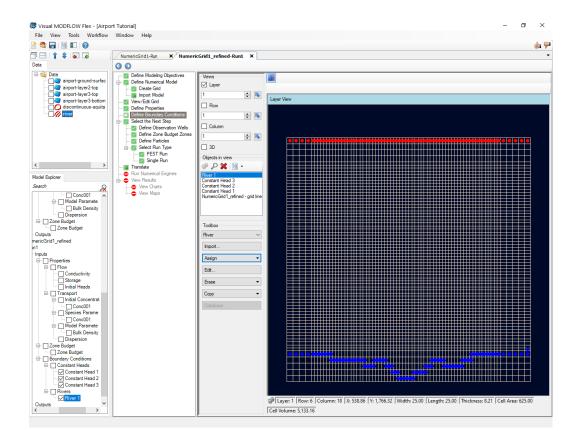
• Now define the values at this end point, in the parameters grid, based on the values below:

River Stage (m)	15.5
Riverbed Bottom (m)	15.0
Conductance (m²/d)	(do not enter any values)
River Width (m)	25
Riverbed Thickness (m)	0.1
Riverbed Conductivity (m/s)	1E-4

- We will now linearly interpolate the intermediate values. To do this:
- Click the grey box next to the top (start) row to highlight the whole row blue as shown below:

۲								Define Bo	undary Condition				-	- 🗆 🛛
Boundary Condition Soript														
Sci	nedule 🗸	Name	River	1			👔 🏠 Calculatio	n 0.0001 √:	x 🏥 🏢 📰 🖍 📳					
	This boundary condition is static. Switch to transient to define a schedule.	Laye	r V	Ro 5	7 Col	umn 🛛	River Stage (m) 🔽	Riverbed Bottom (m 🕁	Conductance (m^2/d 🛛	Conc001 (mg/L 🔻	River Width (😽	Riverbed Thickness (∇	Riverbed Kz (m/ 😽	Active 🔽 🔨
		- F - 1					16	15.5			25		0.0001	v
80		1	1	67	2					-1				v
		1	1	67	3					-1				~
		1	1	67	4					-1				✓

- Holding the CTRL key on your keyboard, click to also highlight the last (end) row.
- Now click the interpolate button []. The intermediate rows should now populate with interpolated values.
- Click **[Finish]** to complete the boundary condition. The polyline will now turn to a set of blue points, indicating that a River boundary condition has been assigned to these cells. The interface should now look like the image below:



Recharge

In many hydrogeologic settings, aquifers are recharged by water infiltrating from the land surface. In order to assign recharge in Visual MODFLOW Flex, you must be viewing the top layer of the model. Check the 'Views' frame in the upper left-hand side of the main workflow window to see which layer you are currently in. The first boundary condition to assign is the recharge flux to the aquifer:

- First, you need ensure you are viewing Layer 1. Type '1' into the [Layer] field under 'Views' (or use the arrow buttons).
- Select 'Recharge' from the list of boundary conditions in the toolbox.
- Click [Assign]>[Entire Layer] from the toolbox. The 'Define Boundary Condition' dialog will appear.
- Click [Next >>] to accept the default name.
- Enter 100 in the 'Recharge (mm/yr)' column and hit F2 to propagate this value to all rows.
- Leave the default value of **-1 for Conc001**; this indicates that no contaminant mass will be assigned to the recharge flux.
- Enter 0.1 in the 'Ponding (m)' column and hit F2 to propagate this value to all rows, as shown below.
- Finally, change the Schedule from 'Transient' to 'Static'
- The Define Boundary Condition window should now look like the image below:

chedule Static 🔹 🛶 🧱	Nan	ne Rec	harge		🛛 🏠 Calculation	n 0.1	\sqrt{x} = =		
This boundary condition is static. Switch to	L	.ayer	▼ Row	▼ Column ▼	Recharge (mm/ 😙	Ponding (m 😽	Conc001 (mg/ 😽	Zone 🛛	Active 🔽
ransient to define a schedule.	•	1	71	1	100	0.1	-1	1	✓
		1	71	2	100	0.1	-1	1	-
		1	71	3	100	0.1	-1	1	✓
		1	71	4	100	0.1	-1	1	<
		1	71	5	100	0.1	-1	1	✓
		1	71	6	100	0.1	-1	1	✓
		1	71	7	100	0.1	-1	1	✓
		1	71	8	100	0.1	-1	1	✓
		1	71	9	100	0.1	-1	1	✓
		1	71	10	100	0.1	-1	1	✓
		1	71	11	100	0.1	-1	1	✓
		1	71	12	100	0.1	-1	1	✓
		1	71	13	100	0.1	-1	1	✓
		1	71	14	100	0.1	-1	1	✓
		1	71	15	100	0.1	-1	1	✓
		1	71	16	100	0.1	-1	1	✓
		1	71	17	100	0.1	-1	1	✓
		1	71	18	100	0.1	-1	1	✓
		1	71	19	100	01	-1	1	J

• Click **[Finish]**. All cells in the top layer will be assigned a recharge rate of 100 (mm/yr). The recharge boundary will be displayed as white dots.

Now you will assign a higher recharge value at the Refueling Area where jet fuel has been spilled on a daily basis. First you need to import a polygon shapefile that delineates this area.

- Click [File]>[Import data...]
- For the Data Type, select 'Polygon' from the drop-down list.
- In the Source File field click the [...] button and navigate to your Public "My Documents" folder, then 'VMODFlex\Tutorials\Airport\suppfiles\refuelling-area.shp', and click [Open]
- Click [Next>>]
- Click [Next>>] (accept the defaults)
- Click [Next>>] (accept the defaults)
- Click [Finish]. You should now see a new data object, 'refuelling-area' appear in the data tree, in the top left corner of the window.
- Click on the box beside this data object in the tree \checkmark . The data object should now appear in the Layer View of the grid (it is located in the top middle of the site).

Please Note: you may need to uncheck 'Recharge' from the Model Explorer tree to make the view less cluttered.

• Zoom into this area (using the mouse wheel, or the Zoom in button on the toolbar).

• Click [Assign]>[Using Data Object...] from the toolbox. A 'Define Boundary

Condition' window will appear. Use the [button to add the **'refuelling-area'** object to the geometry section of the dialog.

- Click [Next >>] to accept the default name.
- Enter 250 in the 'Recharge (mm/yr)' column and hit F2 to propagate this value to all rows.
- Enter 0.1 in the 'Ponding (m)' column and hit F2 to propagate this value to all rows.
- Finally, change the Schedule from 'Transient' to 'Static'
- Notice that Conc001 has a default of -1 indicating that there is no defined mass flux assigned to this boundary condition. You will modify this later on in the Transport section of the tutorial.

chedule Static 🔹 🗰 🧱	Name	Rechar	ge		🛛 🏠 Calculation	0.1	\sqrt{x} \blacksquare \blacksquare		
This boundary condition is static. Switch to	Laye	er 🛛	Row 🛛	Column 🗸	Recharge (mm/ 😽	Ponding (m 🝸	Conc001 (mg/ 😽	Zone 🛛	Active 🗸
ransient to define a schedule.	· · ·		9	23	250	0.1	-1	2	✓
	1		9	24	250	0.1	-1	2	✓
	1		9	25	250	0.1	-1	2	✓
	1		9	26	250	0.1	-1	2	✓
	1		9	27	250	0.1	-1	2	✓
	1		8	23	250	0.1	-1	2	✓
	1		8	24	250	0.1	-1	2	✓
	1		8	25	250	0.1	-1	2	✓
	1		8	26	250	0.1	-1	2	✓
	1		8	27	250	0.1	-1	2	<
	1		7	23	250	0.1	-1	2	✓
	1		7	24	250	0.1	-1	2	✓
	1		7	25	250	0.1	-1	2	✓
	1		7	26	250	0.1	-1	2	 ✓
	1		7	27	250	0.1	-1	2	✓
	1		6	23	250	0.1	-1	2	₹
	1		6	24	250	0.1	-1	2	✓
	1		6	25	250	0.1	-1	2	✓
	1		6	26	250	01	-1	2	J

- Click [Finish]. You should now see a new zone of cells colored blue, indicating the new RechargeZone2, with this new value
- Click [Database] to see the recharge zones you created, and their corresponding values.

>		Recharge Attribute Info											
	Zone	Color	Rate (mm/yr)	Ponding Depth (m)	Conc001 (mg/L)								
•	1		100	0.1	-1								
	2		250	0.1	-1								
	_	_	_										
				OK	Cancel								

- Click [OK] to close the window
- Now is a good time to save the project. Click [File]>[Save Project] from the main menu.

Define Pumping Wells

To generate a pumping well boundary condition, you can either add them one at a time through the user interface, or use a wells data object for this model, you will begin by importing a wells data object.

- Click [File]>[Import Data...] from the main menu.
- Select 'Well' as the data type.
- [...] to choose the source file
- Browse to your Public "My Documents" folder, then 'Visual MODFLOW Flex\Tutorials\Airport\suppfiles**Pumping_Wells.xlsx'** file.
- [Open]
- [Next>>]. The next window will show a preview of the data to be imported.

۲				Data I	Import				×
W	ork sheet and range -								
	Select Worksheet				From row				
	Sheet1\$			~	1	-			
	eview Source Data								
FR	Row	Well Id	Х	Y	Elevation	Well bottom	Screen Id	Screen top Z	~
J		Supply Well 1	1415	535	18.5	0	1	5	
.0		Supply Well 2	1463	509	18.4	0	1	5	+
									_
									\sim
<									>
					[< <back< td=""><td>Vext >> Can</td><td>cel Help</td><td></td></back<>	Vext >> Can	cel Help	
					L				

- [Next>>].
- VMOD Flex provides you with various options to import well data. In this window, you must select to import the well heads, screens, and pumping schedules.
- Select the [Well heads with the following data] check box.
- Select the [Pumping Schedule] check box.

🕽 Data Import				_		\times
Select the format of the vertic	al data in your data so	irce				
Non-vertical Wells	Elevation	O Measured depths				
Time						
Absolute						
◯ Relative						
Select the type of data you w	ant to import					
O Well heads only with Id, s	к, y, Elevation and dep	h				
Well heads with the follow	wing data					
Screens (ID, location	ns)					
Pumping sched	lule Well Mo	el: WEL ~				
Observation points						
Observed head						
Observed cond Target residual						
O Well tops	~					
U vvei tops						
		<<	Back Next >>	Cancel	Help	0

- [Next>>]
- [Next>>] to accept the default Coordinate System.

The following 'Data Import' window will then appear:

 Wel X Y Elev 	Screens Pump Target fields II Id	Schedule Map to Well Id X Y Elevation	Unit cate None Length Length Length	gory None m m	Unit 1		Data Type Text Numeric Numeric
 X Y Elev 	II Id	Well Id X Y	None Length Length	None m	1		Text Numeric
 X Y Elev 	vation	X Y	Length Length	m	1		Numeric
• Y • Elev		Y	Length		-		
* Elev			-	m	1		M
		Elevation	Length				Numeric
* Wel	II bottom		Lengui	m	1		Numeric
		Well bottom	Length	m	1		Numeric
Well	lld	X Y	Elevation	Well bottom	Screen Id	Screen top Z	Screen bottom Z
Supply V	Well 1 1415	535	18.5	0	1	5	3
Supply V	Well 2 1463	509	18.4	0	1	5	3

In this screen, you need to map the fields from the spreadsheet to required fields in the data import utility. If you prepare your Excel file with the exact column names that are expected by Visual MODFLOW Flex, then no mapping is required and this can save you time. For this exercise, the source Excel file has the map names pre-defined. Take a moment to review the required fields for the Wells import:

- Well heads: Well ID, XY Coordinates, Elevation, and Bottom
- Screens: Screen Id, Screen top Z, Screen bottom Z
- Pump Schedule: Pumping start date, Pumping end date, Pumping rate

When working with your own pumping well data for your models, you can use this Excel file as a template – having all the fields automatically mapped for you reduces the effort required during the import process, and minimizes sources of error.

Switch to the Screens Tab to see the mapped fields:

I Text 1 Numeric 1 Numeric 1 Numeric	None None 1 Text Length m 1 Numeric Z Length m 1 Numeric	-		eads Screens	jet fiel				_	-	-	T	_	_		Map to		_		Unit cat	enory			1	Jnit			 Multipl	er			Data	а Туре	
I Numeric Screen Id Screen top Z Screen bottom Z 1	Z Length m 1 Numeric Image: Second Secon	1	•	Screen Id	jor noi	Inordo				_	_	1	Sci	reer		iup ii		_	Non		.ogory		None				1	Turupi		Te	ext	Dut	11700	
Screen Id Screen top Z Screen bottom Z 1 5 3	Elevation Well bottom Screen Id Screen top Z Screen bottom Z 18.5 0 1 5 3	ŀ	•	Screen top Z								-	Scr	reer	n top	νZ			Leng	th			m				1	 		Nu	Imer	ic		
1 5 3	18.5 0 1 5 3		•	Screen botto	m Z	2						-!	Sc	reer	n bo	ttom 2	z		Leng	th			m				1			Nu	Imer	ic		
1 5 3	18.5 0 1 5 3	_ `	quin >	ired																														
		•) 2e [X Data Preview	1					×						Y			F	wation		Well	bottom			Scree	1 Id	Ser	en ton	7		Cree	n hotte	m 7
1 5 3		urc	י כפ [\	×	141	1415	115	15		×				53	35	Y				evation		Well	bottom			Scree	ı Id		en top	Z	_	òcree	n botto	m Z
53		Req F) 2e [X Data Preview	1									1																_				

• Click [Next>>].

The Data Import preview will appear:

				[Data Import				- 🗆 🛛
Errors and	d warnings ads 🔗 Screer	ns 📀 Pump Sche	dule						
	9 5000								
🗌 Do n	ot import rows wi	th warnings							
		-							
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01 02		Supply Well 1	1415 1463	535 509	18.5 18.4	0		-	
./ 2		Supply Well 2	1463	505	10.4	0]	
<									
·									-
						< <ba< td=""><td>ck Finish</td><td>Cancel</td><td>Help</td></ba<>	ck Finish	Cancel	Help

- You should see a series of green check marks next to the 'Heads', 'Screens' and 'Pump Schedule' tabs indicating that there were no import errors.
- Click [Finish].

The **'Pumping_Wells'** will now appear as a new data object in the Data tree.

Next, you need to add the imported wells to the Numerical Model

- At the Define Boundary Conditions step in the workflow, under Toolbox, choose **'Wells'** from the first dropdown menu listing available boundary condition types.
- Click the [Assign]>[Using Data Object] button. An 'Add Wells' window will appear.
- Select (highlight) the 'Pumping_Wells' data object from the Data Tree (you may need to move the Pumping Wells Boundary Condition dialog to the right in order to see this).
- Click [button located in the middle of the 'Create Well Boundary Condition' window, under 'Select Raw Wells Data Object or Drag & Drop'. Once completed, your display should appear as shown below.

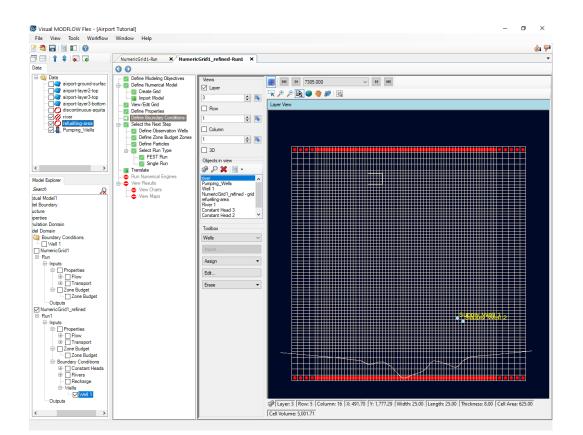
۲	Add	Wells												- 0	×
Sele	ct Rav	t Name: Well 1 v Wells Data Obje mping_Wells	ect or Drag & Drop	•		Well Mo	del: WEL 🗸	Data T Screet	o Display Active We Is	ell: <none></none>				Isplay Format Elevation Measured D	lepths
Vert	_	mping_vveiis				Find:								-	
	ell Hea							Scree							
ľ	•	•• × •• f	a 15 1						🖡 🗰 🗱 🛍 💼	Ta	op (m)		Bottom ((m)	
IC.		Name	x	Y	Zmax	Zmin	Active		1	5	ab (m)		3	111)	
ŀ		Supply Well 1	1415	535	18.5	0									
		Supply Well 2	1463	509	18.4	0									
								Pump	ow as Relative Times ng Schedule P IIII 🗱 🗱 🖄 🖺		ie 1/1/2000 12:00				
									Start 0.000	End 7305.00		Rate (m^3/d)	0	ionc001	
											-	Apply		ĸ	ancel

• Click [OK]. The pumping wells have now be added to the numerical model.

You should see a new node appear on the Model Explorer, under

'NumericGrid1_refined/Run/Inputs/Boundary Conditions/Wells'. In order to see these wells, you need to turn off the Recharge coverage and change to Layer 3.

- Click on the box beside 'Recharge' in the Model Explorer, to remove the check box
- Change to Layer 3 (as explained earlier).
- Also, you may need to zoom out to the full grid extents, by selecting the [] (Zoom to Full Extents) button on the toolbar above the grid.
- You should see the two points representing the wells, located in the lower right corner of the model domain, as shown in the following figure.



 Now is a good time to save the project. Click [File]>[Save Project] from the main menu.

Define Head Observations

Field observations of groundwater heads and fluxes are essential in order to calibrate the results obtained by MODFLOW. In this exercise, you will add several head observations wells, and analyze these against the corresponding calculated values after the model run is complete. The head observations are grouped into two files, one for layer 1 (observation wells 1-5) and another for layer 3 (observation wells 6-10). First we need to import the observation wells:

- Click [File]>[Import Data] from the main menu bar
- Ensure 'Well' is selected as the Data Type
- [...] to choose the source file.
- Browse to your Public 'My Documents' folder, then 'Visual MODFLOW Flex\Tutorials\Airport\suppfiles\Head_Observations_Layer1.xlsx' file.
- [Open]
- [Next>>]

A preview window will appear displaying the source data.

,	Data Import								_		×
Wo	rk sheet and rang	e									
5	elect Worksheet					From row					
	Observation_Well	s\$		\sim		1	•				
Pre	view Source Data										
	Row	Well Id	X	Y	EI	evation	Well bottom	Logger Id		Logger Z	~
1	1	OW-1	285.5407047387	1622.600243013	20		0	1	17	22	
	2	OW-2	1338.274605103	1476.792223572	20		0	1	17		
J	3	OW-3	358.4447144592	747.7521263669	20		0	1	17		-
I	4	OW-4	1125.394896719	476.5492102065	20		0	1	17		-
J	5	OW-5	912.5151883353	1103.523693803	20		0	1	17		
L .								_			\sim
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									_		_
							< <back< td=""><td>Next >> (</td><td>Cancel</td><td>Help</td><td>D</td></back<>	Next >> (Cancel	Help	D

- [Next>>]. VMOD Flex provides you with various options to import well data.
- Choose the radio button [Well heads with the following data]
- Then select [Observations points]
- Then select [Observed heads]
- Ensure you have the options selected as shown below.

Image: Select the format of the vertical data in your data source Image: Non-vertical Wells Image: Select the format of the vertical data in your data source Image: Select the type of data you want to import Image: Select the type of data you want to import Image: Select the type of data you want to import Image: Select the type of data you want to import Image: Select the type of data you want to import Image: Select the type of data you want to import Image: Select the type of data you want to import Image: Select the type of data you want to import Image: Select the type of data you want to import Image: Select the type of data you want to import Image: Select the type of data you want to import Image: Select the type of data you want to import Image: Select the type of data you want to import Image: Select the type of data you want to import Image: Select the type of data you want to import Image: Select the type of data you want to import Image: Select the type of data you want to import Image: Select the type of data you want to import Image: Select the type of data you want to import Image: Select the type of data you want to import Image: Select the type of data you want the following data Image: Select the type of data you want the following data Image: Select the type of data you want the following data <th></th> <th></th> <th></th> <th></th> <th></th> <th></th>						
Non-vertical Wells ● Bevation Measured depths Time ● Absolute ● Relative Select the type of data you want to import ○ Well heads only with Id, x, y. Bevation and depth ● Well heads with the following data ○ Screens (ID, locations) ● Pumping schedule Well Model: ● Observation points ● Observation points ● Observation points ● Target residuals ● Well tops	🝔 Data Import			_		\times
Time	- Select the format of the verti	ical data in your data so	urce			
Absolute Relative Select the type of data you want to impot Well heads only with Id. x. y. Elevation and depth Well heads with the following data Screens (ID, locations) Pumping schedule Well Model: WEL Observed heads Observed concentrations Target residuals Well tops	Non-vertical Wells	Elevation	O Measured depths			
 Relative Select the type of data you want to impot Well heads only with ld, x, y. Elevation and depth Well heads with the following data Screens (ID, locations) Pumping schedule Well Model: WEL Observation points Observed heads Observed concentrations Target residuals Well tops 	Time					
Select the type of data you want to impot Well heads only with Id, x, y, Elevation and depth Image: Well heads with the following data Screens (ID, locations) Pumping schedule Well Model: Image: Well Model WEL Image: Well Model WEL Image: Well Model WEL Image: Well Model WEL Image: Well heads Observed heads Image: Observed concentrations Target residuals Image: Well tops Well tops	Absolute					
 Well heads only with Id, x, y, Elevation and depth Well heads with the following data Screens (ID, locations) Pumping schedule Well Model: WEL Observation points Observed heads Observed concentrations Target residuals Well tops 	O Relative					
 Well heads with the following data Screens (ID, locations) Pumping schedule Well Model: WEL Observation points Observed heads Observed concentrations Target residuals Well tops 	Select the type of data you	want to import				
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Pumping schedule Well Model: WEL Observation points Observed heads Observed concentrations Target residuals Well tops	Well heads with the following the followi	owing data				
 Observation points Observed heads Observed concentrations Target residuals Well tops 	Screens (ID, location)	ons)				
Observed heads Observed concentrations Target residuals Well tops	Pumping sche	dule Well Mod	el: WEL \sim			
Observed concentrations Target residuals O Well tops	Observation points					
Target residuals Well tops	Observed heat	ads				
O Well tops	~					
	Target residua	als				
< <back next="">> Cancel Help</back>	 Well tops 					
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< <back next="">> Cancel Help</back>						
			< <back next=""></back>	>> Cancel	Help	p

- [Next>>]
- [Next>>] to accept the default Coordinate System

In this screen, you need to map the fields from the spreadsheet to required fields in the Wells Import utility.

	Tar	rget fields	Map to	Unit cate	20D/	Unit	Multiplier	Data Type
•	Well Id	gerneids	Well Id	None	None	onn	1	Text
-			X	Length	m		1	Numeric
-			Y	Length	m		1	Numeric
-	Elevation		Elevation	Length	m		1	Numeric
-	Well bottom		Well bottom	Length	m		1	Numeric
	ired							
ce	-	×	Y	Elevation	Well bottom	Logger Id	Logger	Z Observed Head
ce	Data Preview Well Id	-		Elevation 20	Well bottom	Logger Id	Logger 17	Z Observed Head
ce	Data Preview Well Id	X 285.540704738 1338.27460510	7 1622.600243013 3 1476.792223572					
ce DW DW	Vell Id V-1 V-2 V-3	X 285.540704738 1338.27460510 358.444714459	1622.600243013 1476.792223572 747.7521263669	20 20 20	0 0 0	1	17 17 17 17	19 18.4 17.6
ce DW DW DW	V-1 V-2 V-4	X 285.540704738 1338.27460510 358.444714459 1125.39489671	1622.600243013 1476.792223572 747.7521263669 476.5492102065	20 20 20 20 20	0 0 0 0	1 1 1 1 1	17 17 17 17 17 17	19 18.4 17.6 16.7
0W 0W 0W	Vell Id V-1 V-2 V-3	X 285.540704738 1338.27460510 358.444714459	1622.600243013 1476.792223572 747.7521263669 476.5492102065	20 20 20	0 0 0	1 1 1	17 17 17 17	19 18.4 17.6
ce DW DW	V-1 V-2 V-4	X 285.540704738 1338.27460510 358.444714459 1125.39489671	1622.600243013 1476.792223572 747.7521263669 476.5492102065	20 20 20 20 20	0 0 0 0	1 1 1 1 1	17 17 17 17 17 17	19 18.4 17.6 16.7

To save time, you can prepare your Excel file with the exact field names that are required by Visual MODFLOW Flex, and then no mapping is required. For this exercise, the source Excel file has the field names pre-defined for automatic mapping and can be used as a template/guide for your other projects. Take a moment to review the required fields for the Wells import:

- Well heads: Well ID, XY Coordinates, Elevation, and Bottom
- Observation points: Logger Id, Logger Z, Head observation date, Observed head
- [Next>>]

The Data Import preview will appear, indicating if there were any errors with the file import. This file should import with no errors.

• [Finish]

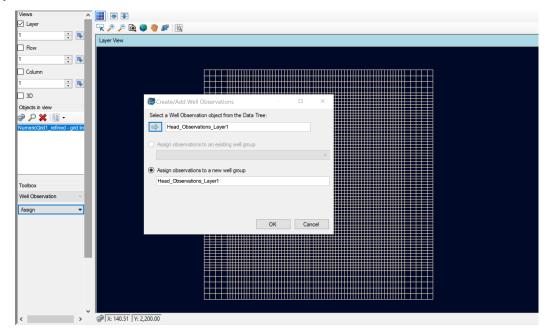
The **'Heads_Observations_Layer1'** will now appear as a new data object in the Data Tree. Take a moment and visualize this in the 3D Viewer.

Next you need to add these raw observation wells as observation points for the numerical model.

- Click [[(Next Step) to proceed.
- Select [Define Observation]
- Next, ensure that 'Well Observation' is selected from the first dropdown menu under the 'Toolbox' section.

- Be sure that the 'Head_Observations_Layer1' data object is selected in the Data Tree.
- Click [Assign]>[Using Data Object] from the toolbox. Click on the [button to add the Well Observation object.
- Ensure you have the options selected as shown below.
- Click **[OK]**. The observation wells will be added to the display and the numerical model tree.

You should see several green points in the model domain that represent the locations where head measurements were taken. Note that all of the head observations added so far are in layer 1.



Now you will repeat these steps to import the observation wells for layer 3 of the model. Follow the same steps above, but this time import the **'Head_Observations_Layer3.xlsx'** file. When you import a second observation group, you will be prompted to assign the observations "...to an existing well group", or to "... a new well group', as indicated in the image below:

Create/Add Well Observations Select a Well Observation object from the Data Tree: Head_Observations_Layer3				
 Head_Observations_Layer3 Assign observations to an existing well group Head_Observations_Layer1 Assign observations to a new well group Head_Observations_Layer3 	💭 Create/Add Well Observations			\times
Assign observations to an existing well group Head_Observations_Layer1 Assign observations to a new well group Head_Observations_Layer3	Select a Well Observation object from the Data Tree:			
Head_Observations_Layer1 Assign observations to a new well group Head_Observations_Layer3 	Head_Observations_Layer3			
Assign observations to a new well group Head_Observations_Layer3	O Assign observations to an existing well group			
Head_Observations_Layer3	Head_Observations_Layer1			\sim
	 Assign observations to a new well group 			
OK Cancel	Head_Observations_Layer3			
OK Cancel				
OK Cancel				
		ОК	Cano	cel

- Click 'Assign observations to a new well group'
- OK

Once the observations for layer 3 have been imported you can view them in layer 3, as shown below:

e View Tools Workflow	Window Help					
3 🔒 💀 🗈 🥝						da da
	NumericGrid1-Run × Numeric	Grid1 refined-Run1 ×				
	9 0					
Data airport-ground-surface airport-layer2-top	Define Modeling Objectives Define Properties Define Boundary Conditions	🗹 Layer	^ IIII (# 19) '''''' (# 19) (# 19) (# 19) (# 19) (# 19) (# 19) (# 19) (# 19) (# 19) (# 19) (# 19) (# 19) (# 19) (# 19) (# 19)			
airport-layer3-top airport-layer3-bottom discontinuous-aquitard	Select the Next Step	3 🕂 🖡	Layer View			
river refuelling-area Pumping_Wells Head Observations Lav		1 💼 K				
Head_Observations_Lay	Image Run Translate Run Numerical Engines	1 🔅 🖡				
>	View Results View Charts View Maps	Objects in view				
Explorer		Head_Observations_Layer1 Head_Observations_Layer3 NumerioGrid1_refined - grid lines		¢.		
Conc001 Model Parameters Dulk Density Dispersion ne Budget		Toolbox				
Dre Budget Cone Budget1 Dundary Conditions Constant Heads		Well Observation · · · Assign · ·			¢.	
Constant Head 1 Constant Head 2 Constant Head 3 Rivers				*		
- River 1 Recharge Wells						
rvations Head_Observations_Lay						
×						

- Now is a good time to save the project. Click [File]>[Save Project] from the main menu.
- Click [] (Next Step) to proceed.

Select Run Type and Engines

At this step in the tutorial, you select which engine(s) to run in the simulations:

- In the 'Select Run Type' step, select [Single Run]
- From the 'Single Run' step in the workflow, you will see 'USGS MODFLOW 2005 from WH' is selected along with 'MT3DMS' as the transport engine.
- For the first run, we will run the flow solution only, without transport.
- De-select the checkbox for 'Run Transport Engine'
- Click [[(Next Step) to proceed.

MODFLOW-2005 Translation Settings

At the Translate step you have the option to adjust the various parameters and flags for the MODFLOW packages and run time settings. Available options include: 'Settings' (General), 'Settings' (MODFLOW-2005), 'Solvers', 'Recharge and Evapotranspiration', 'Lake', 'Layers', 'Rewetting', 'Initial Heads', 'Anisotropy', 'Output Control' and 'Advanced Settings'.

- Select [MODFLOW-2005]>[Settings]
- Enter 7300 for 'Steady-State Simulation Time' (in the grid in the main window).

Settings General General General			
	gs		
Settings Property Package LPF MODFLOW-2005 Run Type Steady-State Solvers Steady-State Simulation Time 7300 Recharge and EVT Lake No Initial Heads Arisotropy Output Control Advanced Settings Steady-State Simulation Time Steady-State Simulation Time Steady-State Simulation Time	Settings ADDFLOW-2005 Solvers Solvers Recharge and EVT Lake Layers Rewetting Initial Heads Anisotropy Output Control	2005 Property Package Run Type Steady-State Simulation Time Save .FLO file sads py Control ed Settings Steady-State Simulation Time	7300

Click [Translate] to create the MODFLOW-2005 packages. Check the log to confirm the translation has finished.

ttings Translati	on Log DIS LPF RIV CHD RCH BAS OC PCG NDC WEL IN	
22:05 PM GMG I	Package	-
22:05 PM	GMG started	
22:05 PM : Initial		
	Aterloo Hydrogeologic	
22:05 PM : Trans		
22:05 PM : Finali 22:05 PM : Finali		
22:06 PM	GMG completed: 'Conceptual Model1.GMG'	
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22:06 PM WHS	Package	
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	ize do Hydrogeologic	
22:06 PM : Trans		
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22:06 PM	WHS completed: 'Conceptual Model1.WHS'	
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22:06 PM : Trans		
22:06 PM : Finali		
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22:06 PM NDC F		
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	y Cell Package translator: Initialize	
22:06 PM No Dry	y Cell Package translator: Finalize	
22:06 PM	NDC completed: 'Conceptual Model1.NDC'	
22:06 PM ####	######################################	
22:06 PM #####	################ MODFLOW-2005 Translation Started ####################################	
22:08 PM	WEL started	
22:08 PM	WEL completed: 'Conceptual Model1.WEL'	
22:08 PM	MNW1 package is not active in the simulation.	
22:08 PM	MNW2 package is not active in the simulation.	
22:08 PM	MNWI package is not active in the simulation.	
	############### MODFLOW-2005 Translation Finished ####################################	
	######################################	
2:08 PM ####	######################################	
	######################################	
22:08 PM	SFR skipped.	
	on a supped.	
2.00 FM #####	With the second se	
22:08 PM NAM F		
22:08 PM	NAM started	
22:08 PM #Nam	e File translator: Initialize	
22:08 PM #Nam	e File translator: Finalize	
22:08 PM	NAM completed; 'Conceptual Model1.MODFLOW.IN'	
	######################################	

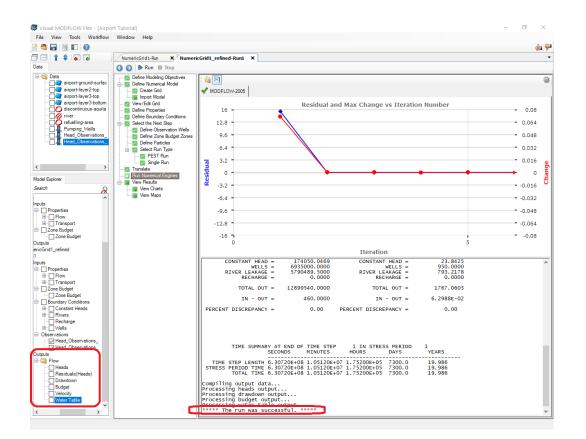
• Click [] (Next Step) to proceed.

Run MODFLOW-2005

At this step in the tutoria,I, you will run the model:

• Click the [Run] button to run MODFLOW-2005.

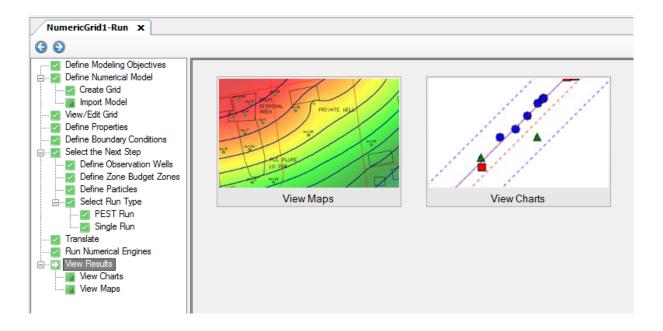
The model run should complete in a few seconds. Once finished, you should see the message: "The run was successful" in the engine progress window. In addition, you will see several items will be added to the model tree under 'Output', as shown below:



- Now is a good time to save the project. Click [File]>[Save Project] from the main menu.
- Click [] (Next Step) to proceed.

View Maps (Heads, Velocities and Calibration Residuals)

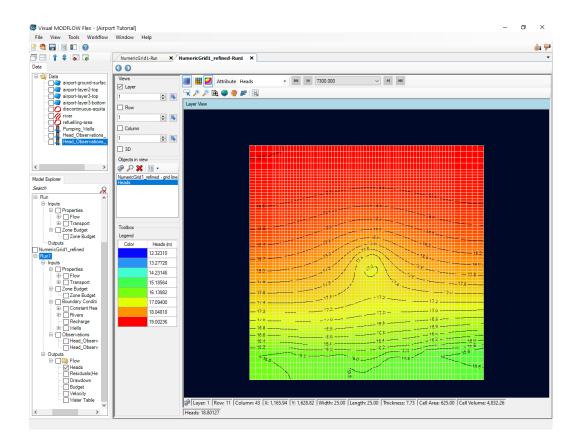
The following 'View Results' window will then appear; you have the option to View Maps or View Charts. We will start by viewing maps of heads.



Heads

The standard display at the View Maps step includes a visualization of the output simulated head distribution. To display the simulated heads do the following:

• Click [View Maps] button to proceed. You will then see color shading of the calculated heads, in layer view. You can press F4 to hide the workflow, and bring it back again at any time by pressing F4 again.



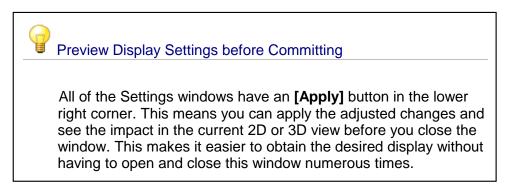
- If you do not like the default contour interval or line color, you can customize the contour map settings.
- To access the contouring options for Heads, **right-click on 'Heads' from the model tree**, and select **[Settings...]**. The following dialog will appear

Settings - Heads (NumericGrid1_refined-Run/ModelRunResult/La	yer View) 🛛 🗖 🛛 🛛
General Info Info Details I · Statistics I · Style	
Type Cell Zone Data Source User created	
Color	
Heads	
Apply OK	Cancel Help

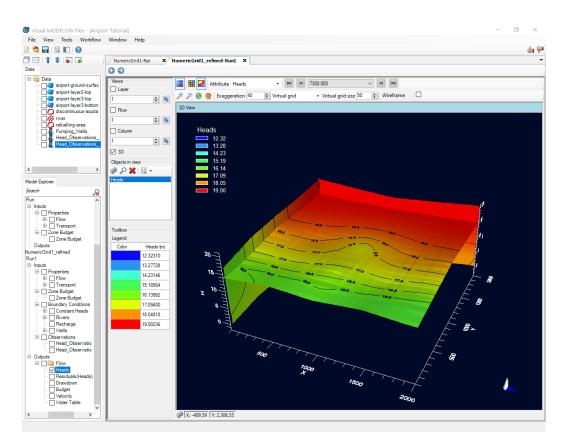
- From the Settings tree on the left, select 'Style' followed by 'Contour Lines'. This will expand the settings window and give you access to the Contour Line settings.
- Under 'Automatic contour', enter 0.5 for the contour interval, and start/finish the contour at 12/20. This is shown below:

Style	Contour Lines			
···· Colors ···· Contour Lines	Show Contour Lines	Heads	Min Value	12.3230962753296
	✓ Show Contour Labels		Max Value	19.0023612976074
	Automatic contour		Custom Contour	
	Contour Interval		Use Custom	Contour Levels
	0.5		New Value	
	Start Contour Value		INEW VAILUE	
	12		Add New	Remove
	Finish Contour Value			
	20			
	Lines style settings		Label settings	
	Line Style		Label Spacing	
		v	100	
	Line Width		Label Margin	
	1	÷	1	
	Color		Number of dec	
	Custom 🗸		3	➡ Label Font

- When you are finished, click [OK].
- This will apply the changes to the head contours in your current view.



 You can also display heads along a row, along a column, or in 3D using the same tools that you used earlier. • In the 'Views' section activate the 3D view and deactivate the layer view. Apply an exaggeration of 40 and reorient your view so that you can see head values along a layer, column and row. You should see something similar to the image below:



• Take a moment to view the heads in other layers/rows/columns.

Velocity Vectors

It is also possible to visualize the results of your flow model as a distribution of velocity vectors, which allows you to easily display and interpret flow fields. To display a velocity map do the following:

- First, ensure you are viewing 'Layer 3'. This layer contains the pumping well, and should contain a significant flow field in that region.
- Turn off the check box beside 'Heads' in the Model Explorer
- Turn on the 'Velocity' output option, in the Model Explorer under 'Outputs' > 'Flow'
- Access the Velocity display settings by right-clicking and selecting 'Settings'
- In the Settings window, access the 'Style' > 'VelocityMap' settings

The VelocityMap settings window should appear as below:

General Style	VelocityMap
···· VelocityMap	Show Show legend
Colors	Show normal velocity color map
	Show isolines
	✓ Show layer 1
	✓ Show row 1 (1-71)
	✓ Show column 1
	Velocity Vectors
	On X 29 🗘 On Y 29 🖨 On Layer 1 🖨
	Color
	Custom O By normal velocity
	Velocity type
	O Darcy Average linear
	Show vectors as
	O Direction Projection Magnitude
	Scale
	Linear Logarithmic
	Scale factor
	1.0 Aax. velocity 4.068

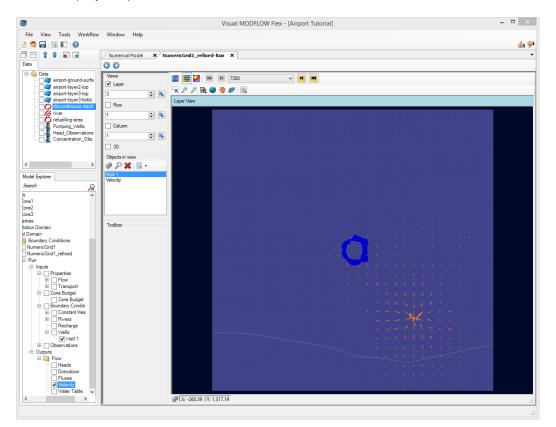
Velocity vectors may be displayed using average linear or Darcy velocities. In-plane velocity vectors can be displayed using the full magnitude of the vector (i.e. the out-of-plane velocity component will be included), as a projection (i.e. only the in-plane velocity component is displayed), or simply a directional indicator (i.e. the size of the arrow is not dependent on the actual velocity). By default, the velocity vectors will initially be displayed as a projection with average linear velocity values, on a linear scale.

A normal velocity color map function is also supported, which allows you to interpret flows perpendicular to the selected layer/row/column (i.e. out-of-plane flow). By default the normal velocity color map will be displayed with a red/blue color scheme, with red areas indicating flow inward (i.e. corresponding to the positive X, Y or Z direction), and blue areas indicating flow outward (i.e. corresponding to the negative X, Y or Z direction). Areas with velocities below the specified in-plane range threshold will be displayed using the specified In-plane

color (which is grey by default). You can find more information about the velocity map display settings in the <u>3D Gridded Data</u> section of this manual.

Update the velocity map settings as follows:

- In the 'Color' frame, select the 'Custom' option, and select 'Orange' as the display color
- In the 'Velocity type' frame, select the 'Average Linear' option
- In the 'Scale factor' frame, type a scale factor of 3.0
- Deselect the 'Show legend' option, so that the legend will be hidden
- Once these settings have been applied, the Layer view should look like the image below (Layer 3)



You should be able to see larger velocity vectors in the bottom-right corner of the model, in the vicinity of the pumping wells. These indicate that groundwater flows are significantly faster in this area relative to the rest of the model domain. You may also notice a 'ring' approximately in the middle of the model. This indicates that there is significant flow perpendicular to layer 3 in this zone. Since the ring is blue, that would indicate flow in the negative Z direction, or downwards from layer 2 and into layer 3.

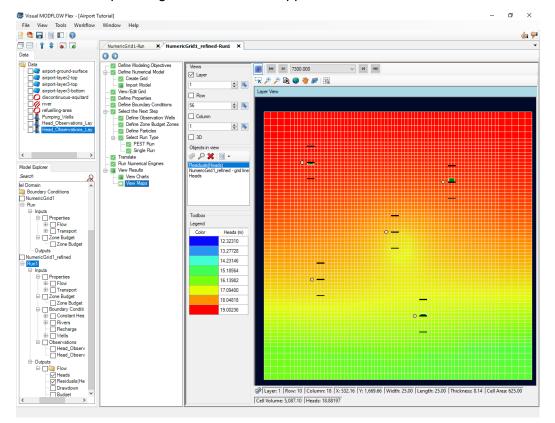
Calibration Residuals

It is also possible to visualize the results of your flow model as a distribution of residuals, provided you have associated observations. This allows you to easily display and interpret

the spatial distribution of the differences between observed and simulated heads. To display a residuals map, do the following:

- First, off the 'Velocity' output option, in the Model Explorer under 'Outputs' > 'Flow'
- Next, turn on the 'Heads' and 'Residuals(Heads) output options, in the Model Explorer under 'Outputs' > 'Flow'

The residuals are shown in the map as a series of error bars. The target residual interval (default = 1 unit of length measurement, typically feet or meters) is shown as a set of three parallel black bars. The residual value is shown as a filled column colored and color coded by whether the residual exceeds the target interval above (blue) or below (red) the observed value or lies within one target interval (green). By default, only the residuals in the current slice (layer/row/column) will be shown. You can experiment with showing residuals differently by changing the ResidualsMap style <u>settings</u>, which can be accessed by right-clicking on the Residuals in the Model Explorer tree.

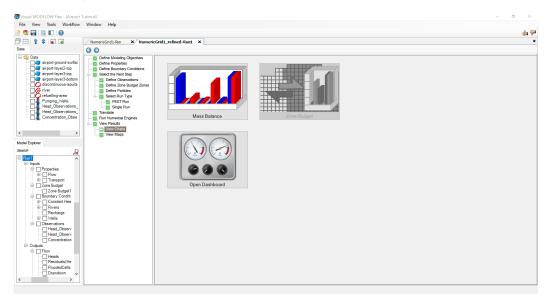


The Residuals Map settings window should appear as below:

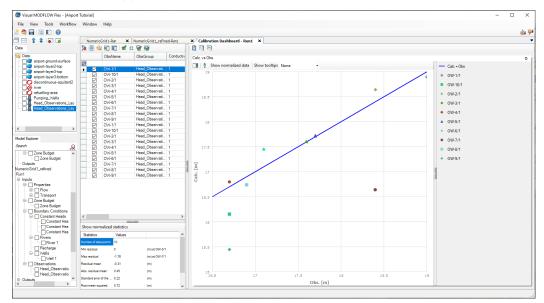
View Charts (Heads)

It's very easy to review calibration charts in Visual MODFLOW Flex whenever observation data has been applied to your model. Since we have applied observed head values in a previous step, we can now proceed to the 'View Charts' workflow step to view the automatically generated calibration charts.

- Click 'View Charts' from the workflow tree. You can open the Mass Balance, Zone Budget, or Open Dashboard at this step. For this tutorial, we will click on Open Dashboard.
- Click [Open Dashboard] to proceed.



As you can see from the image below, Visual MODFLOW Flex supports a number of methods for selecting different wells and provides flexible settings to show/hide wells using filters in the observation data table (show in red below), such as: model layer, observation groups, conductivity zone. Data on the dashboard chart(s) are automatically updated and displayed based on the applied filters.



Next, apply a filter to the model layers so that only observations in Layer 1 are shown:

- Select the dropdown button in the first row of the table for the Layer field and click [[] to select a filter from the Attribute Table. Note, you may wish to expand the table by clicking and dragging the separation line between the table and the chart to the right.
- Deselect the checkbox next to '3' and click **[OK]** and the graph and the statistical values will update.

	♥ ObsName	ObsGroup	ConductivityZone	Lay	/er		Species	Time[day]	Unit
		(Custom)			\sim	M			
	OW-1/1	Head_Observati	1	1		,	Clear Filter		
\checkmark	OW-10/1	Head_Observati	1	3					
\checkmark	OW-2/1	Head_Observati	1	1			Number Filters		•
\checkmark	OW-3/1	Head_Observati	1	1					
\checkmark	OW-4/1	Head_Observati	1	1			(All)		
\checkmark	OW-5/1	Head_Observati	1	1	1		(Blanks)		
\checkmark	OW-6/1	Head_Observati	1	3					
\checkmark	OW-7/1	Head_Observati	1	3					
\checkmark	OW-8/1	Head_Observati	1	3					
\checkmark	OW-9/1	Head_Observati	1	3					
\checkmark	OW-1/1	Head_Observati	1	1					
\checkmark	OW-10/1	Head_Observati	1	3					
\checkmark	OW-2/1	Head_Observati	1	1					
\checkmark	OW-3/1	Head_Observati	1	1					
\checkmark	OW-4/1	Head_Observati	1	1			OK	0	ancel
\checkmark	OW-5/1	Head_Observati	1	1		_			
\checkmark	OW-6/1	Head_Observati	1	3		-	Head	7300	m
\checkmark	OW-7/1	Head_Observati	1	3			Head	7300	m
\checkmark	OW-8/1	Head_Observati	1	3			Head	7300	m
	OW-9/1	Head Observati	1	3			Head	7300	m

Take a moment to experiment with the filters.

To clear the applied filters:

- Click the [127] button in a given field to clear the filter for that field only or click the [127] button in the far left column to clear all filters.
- Now is a good time to save the project. Click [File]>[Save Project] from the main menu.

In the next section of the tutorial, you will define the inputs for the transport run (properties and boundary conditions), then run MT3MDS along with MODFLOW-2005, and view and interpret the results.

Define Transport Model Objectives

The following section outlines the steps necessary to complete a simplified transport model. Similar to a groundwater flow model, a contaminant transport model requires properties (including initial concentrations), boundary conditions (sinks/sources), and observations (in order to calibrate the transport model run against observed field conditions). The steps associated with these model components are described in this and subsequent sections in this tutorial. In this example, the main transport processes that will be simulated are advection (which is defined using the results of the flow model), dispersion, and sorption of a single dissolved species (JP-4, a compound used as jet fuel).

Sorption

For the purposes of this example, the sorption process will be simulated using the (reversible) linear equilibrium sorption model with a single parameter zone for the whole model domain. Note that depending on the complexity of the sites/projects you may deal with, your model(s) may have require multiple zones with different sorptive and reactive properties (such as distribution coefficients, decay coefficients, and yield coefficients) for each dissolved species in the model. In Visual MODFLOW Flex, the properties and processes for the transport model are assigned using the same types of graphical tools as you used for assigning the flow model properties.

For this tutorial you will not need to modify the Distribution Coefficient value you defined during the transport model setup, but you may examine the sorption parameter values as follows.

- From the workflow tree, click on [Define Properties] to go back to this step.
- Under the toolbox, choose [Species Parameter Conc001] from the first menu.
- Click on the [Zone] button and change it to [Kd].

The default distribution coefficient (Kd = 1.0E-7 L/mg) was specified during the setup of the transport numeric engine. If this is not so (e.g. if you did not enter this value when creating the project), enter this now using the **[Edit]** button.

- With 'Species Parameter Conc001' and 'Kd' selected in the toolbox, click the [Edit] button.
- This will open the 'Edit property' window.
- Under the 'Kd' column enter 1E-07 in the first row and click F2 to propagate this value to the rest of the column.

The Kd values for each zone can be modified to accommodate heterogeneous soil properties and reactions throughout the model domain. However, for this example you will keep it simple and use a uniform Distribution Coefficient for each layer of the model.

Dispersion Coefficients

The next step is to define the dispersion properties for the model. Visual MODFLOW Flex automatically assigns a set of default values for each of the dispersivity variables. The following table summarizes the default values.

Longitudinal Dispersivity	10
Horizontal to Longitudinal Ratio	0.1
Vertical to Longitudinal Ratio	0.01
Molecular Diffusion Coefficient	0.0

It is possible to assign alternate values for the longitudinal dispersivity by using the **[Assign]** option buttons from the toolbox. However, for this example, you will use a uniform dispersion value for the entire model domain. In order to modify the horizontal or vertical dispersivity ratios and/or the molecular diffusion values you need to load the Layer Options:

- Right-click on 'Dispersion' from the Model Explorer, under Inputs/Properties/Transport
- Select 'Dispersion Parameters'. The following window will appear:

۲		Dispersion	Parameters	- 🗆 🗙
	📰 🗊 💼			
	Layer	Horiz/Long Dispersivity	Verti/Long Dispersivity	Diffusion Coeff. (m^2 / day)
•	1	0.1	0.01	0
	2	0.1	0.01	0
	3	0.1	0.01	0
				OK Cancel

These parameters can be modified on a "per-layer" basis. For this example, you will not need to modify the defaults.

- Click [Cancel] to close this window
- Now is a good time to save the project. Click [File]>[Save Project] from the main menu.
- Click [[] (Next Step) to proceed

Define Transport Boundaries (Sinks/Sources)

In this section you will define the location and concentration of the contaminant source. The source of contamination will be designated at the refueling area as a Recharge Concentration that serves as a source of contamination to infiltrating precipitation.

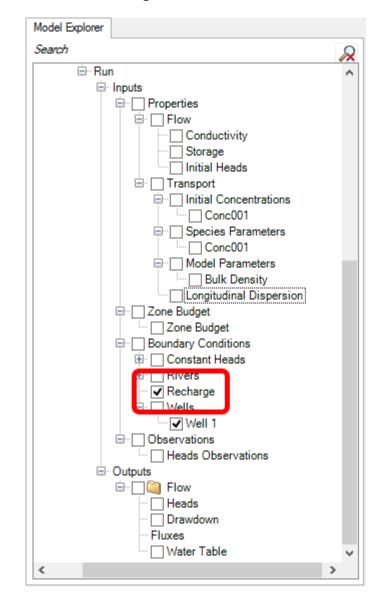
Assign Species Concentrations for the Recharge Boundary

When you defined the flow model, you created a separate recharge zone that covers the refueling area. Now you will add a defined species concentration to this recharge flux:

- Ensure you are viewing the 'Define Boundary Conditions' workflow step.
- Check to ensure that you are viewing Layer 1.
- Select 'Recharge' from the list of available boundary conditions under the toolbox.

You will recall there were two recharge zones created for the flow model: background recharge of 100 mm/yr covering the entire model top, and a small area over the refueling area with a higher recharge rate of 250 mm/yr. The JP-4 source area will be assigned only to this smaller recharge zone.

- If not already visible, you must make the Recharge zones visible. In the Model Explorer, locate the 'Recharge' node, under 'Inputs'>'Boundary Conditions', as shown below.
- Click on the box beside 'Recharge' in the tree



- The recharge cells should now appear in the layer view of the grid
- Under the 'Toolbox' section, click the [Database] button and the following window will appear.

	Zone	Color	Rate (mm/yr)	Ponding Depth (m)	Conc001 (mg/L)
1			100	0.1	-1
2			250	0.1	-1

When the recharge zones were previously created, the values for the chemical species (Conc001) were left as undefined, indicated by -1. You will modify this for the smaller recharge area.

- Locate **Zone2** (the second row in the table)
- Enter 5000 for Conc001 (thereby replacing the -1 value).
- Click [OK] to close the Database window
- Now is a good time to save the project. Click [File]>[Save Project] from the main menu.
- Click [] (Next Step) to proceed
- Select [Define Observations]

Define Concentration Observations

The final step before running the transport simulation is to add the three observation wells to the model to monitor the jet fuel concentrations at selected locations down-gradient of the refueling area. The first observation well (OW1) was installed immediately down-gradient of the refueling area shortly after the refueling operation started. The other two observation wells (OW2 and OW3) were installed two years later when elevated JP-4 concentrations were observed at the first well (OW1).

You will import the concentration observations from an Excel file.

- Click [File]>[Import Data] from the main menu bar
- Ensure 'Well' is selected as the Data Type
- [...] to choose the Source File.
- Browse to your Public 'My Documents' folder, then 'Visual MODFLOW Flex\Tutorials\Airport\suppfiles\Concentration_Observations.xlsx' file.
- [Open]
- [Next>>]

A preview window will appear displaying the source data.

	Sheet1\$			¥	1				
Pre	eview Source Dat								
_	Row	Well ID	X	Y	Logger Z	Logger Id	Chemical	Concentration	1
Ø		OW1	760	1640	16.5	A	Conc001	0	4
Ø	2	OW1	760	1640	16.5	A	Conc001	80	4
Ø	3	OW1	760	1640	16.5	A	Conc001	670	4
Ø	4	OW1	760	1640	16.5	A	Conc001	1120	4
Ø	5	OW1	760	1640	16.5	A	Conc001	1400	4
Ø	6	OW1	760	1640	16.5	A	Conc001	1800	
Ø	7	OW2	810	1415	16.5	Α	Conc001	0	
Ø	8	OW2	810	1415	16.5	Α	Conc001	1	T
Ø	9	OW2	810	1415	16.5	Α	Conc001	5	Т
Ø	10	OW2	810	1415	16.5	Α	Conc001	20	T
Ø	11	OW2	810	1415	16.5	A	Conc001	60	T
Ø	12	OW3	910	1140	16.5	A	Conc001	0	T
Ø	13	OW3	910	1140	16.5	Α	Conc001	0	Ť
Ø	14	OW3	910	1140	16.5	Α	Conc001	0	Ť
Ø	15	OW3	910	1140	16.5	Α	Conc001	0	Ť,
c									>

- [Next>>]
- VMOD Flex provides you with various options to import well data.
- Choose the radio button [Well heads with the following data] radio button
- Then select [Observations points]
- Then select [Observed concentrations]

🐯 Data Import				_		\times
- Select the format of the vertica	al data in your data sou	ce				
Non-vertical Wells	Elevation	○ Measured depths				
Time						
Absolute						
◯ Relative						
Select the type of data you wa	ant to import					
O Well heads only with Id, x	y, Elevation and dept					
Well heads with the follow	ing data					
O Screens (ID, locations)	s)					
Pumping schedu	ile Well Mod	WEL 🗸				
Observation points						
Observed heads						
Observed conce Torrect arciduals						
Target residuals						
Well tops						
			< <back next="">></back>	Cancel	Help	p

- Click [Next>>] to proceed to the Coordinate System step
- Click [Next>>] to accept the default Coordinate System and proceed to the Data Mapping step.
- In this screen, you need to map the fields from the spreadsheet to required fields in the Dells Import utility. To save time, you can prepare your Excel file with the exact filenames that are required by VMOD Flex, and then no mapping is required. For this exercise, the source Excel file has the map names pre-defined. Take a moment to review the required fields for the Wells import:
 - o Well Heads: Well ID, X/Y Coordinates, Elevation, and Well Bottom
 - Observation Points: Logger Id, Logger Z, Concentration observation date, Observed concentration

					Data	Import			-	
	a Mapping		7							
We	I heads Obser	vation Points								
	Target fie	ds	I	Map to	Unit category	Unit		Multiplier	Data Type	• •
	Well Id		Well ID		None	None	1		Text	
	х		х		Length	m	1		Numeric	
	Y		Y		Length	m	1		Numeric	
	Elevation		None		Length	m	1		Numeric	
►	Well bottom		None		Length	m	1		Numeric	
-	• 🗙									
Sou	irce Data Previe	w								
Sou	irce Data Previe Well ID	w	x	Y	Logger Z	Logger Id	Chemica	al Concen	tration Conce	ntration obse
Sou		w 760	X	Y 1640	Logger Z 16.5	Logger Id	Chemica Conc001	al Concen		ntration obse ^
	Well ID OW1 OW1	760 760	x	1640 1640	16.5 16.5	A A	Conc001 Conc001	0 80	2000-01	-01T00:00:0 2-31T00:00:0
	Well ID OW1	760	X	1640	16.5	А	Conc001	0	2000-01	-01T00:00:0

• Click [Next>>] and the the Data Import preview will appear:

and summir				Data Import			
rors and warnings							
🖉 Heads Ob	s Points						_
Do not import row	s with warnings						
	o man manningo						
							_
lapped Data Preview	w						
leads Obs Points							
Row	Well Id	Х	Y	Elevation	Well bottom	Errors	-
Row	Well Id OW1	X 760	Y 1640	Elevation 16.5	Well bottom 15.5	Errors	
Row / 1						Errors	
Row	OW1	760	1640	16.5	15.5	Errors	
Row Ø 1 Ø 2 Ø 3	OW1 OW1	760 760	1640 1640	16.5 16.5	15.5 15.5	Errors	
Row Ø 1 Ø 2 Ø 3 Ø 4	0W1 0W1 0W1	760 760 760	1640 1640 1640	16.5 16.5 16.5	15.5 15.5 15.5	Errors	
Row	0W1 0W1 0W1 0W1	760 760 760 760	1640 1640 1640 1640	16.5 16.5 16.5 16.5	15.5 15.5 15.5 15.5 15.5	Errors	
Row	0W1 0W1 0W1 0W1 0W1 0W1	760 760 760 760 760	1640 1640 1640 1640 1640	16.5 16.5 16.5 16.5 16.5 16.5 16.5	15.5 15.5 15.5 15.5 15.5 15.5 15.5 15.5	Errors	
Row	0W1 0W1 0W1 0W1 0W1 0W1 0W1	760 760 760 760 760 760 760	1640 1640 1640 1640 1640 1640	16.5 16.5 16.5 16.5 16.5	15.5 15.5 15.5 15.5 15.5 15.5	Errors	>
Row Ø 1 Ø 2 Ø 3 Ø 4 Ø 5 Ø 6 Ø 7	0W1 0W1 0W1 0W1 0W1 0W1 0W1	760 760 760 760 760 760 760	1640 1640 1640 1640 1640 1640	16.5 16.5 16.5 16.5 16.5 16.5 16.5	15.5 15.5 15.5 15.5 15.5 15.5 15.5 15.5	Errors	>
Row Ø 1 Ø 2 Ø 3 Ø 4 Ø 5 Ø 6 Ø 7	0W1 0W1 0W1 0W1 0W1 0W1 0W1	760 760 760 760 760 760 760	1640 1640 1640 1640 1640 1640	16.5 16.5 16.5 16.5 16.5 16.5 16.5	15.5 15.5 15.5 15.5 15.5 15.5 15.5 15.5	Errors	>
Row Ø 1 Ø 2 Ø 3 Ø 4 Ø 5 Ø 6 Ø 7	0W1 0W1 0W1 0W1 0W1 0W1 0W1	760 760 760 760 760 760 760	1640 1640 1640 1640 1640 1640	16.5 16.5 16.5 16.5 16.5 16.5 16.5	15.5 15.5 15.5 15.5 15.5 15.5 15.5 15.5	Errors	>
Row Ø 1 Ø 2 Ø 3 Ø 4 Ø 5 Ø 6 Ø 7	0W1 0W1 0W1 0W1 0W1 0W1 0W1	760 760 760 760 760 760 760	1640 1640 1640 1640 1640 1640	16.5 16.5 16.5 16.5 16.5 16.5 16.5	15.5 15.5 15.5 15.5 15.5 15.5 15.5 15.5	Errors	>

• [Finish]

The **'Concentration_Observations'** will now appear as a new data object in the Data tree, as shown below.

Data	
	Data
	🗌 🤕 airport-ground-surface
	🗌 刁 airport-layer2-top
	🗌 🤕 airport-layer3-top
	🗌 🤕 airport-layer3-bottom
	- 🗌 📿 discontinuous-aquitard
	river
	refuelling-area
	Pumping_Wells
	Head_Observations_Layer1
	Head_Observations_Layer3
· ···	Concentration_Observations

Now you need to add these raw observation wells as observation points for the numerical model.

- Ensure that you are on the 'Define Observation' step in the numerical modeling workflow.
- Be sure that the **'Concentration_Observations'** data object is selected in the tree
- Next, ensure that 'Well Observation' is selected from the first dropdown menu under the 'Toolbox' section.

- Click [Assign]>[Using Data Object] from the toolbox. Click on the [button to add the Well Observation object.
- A window will appear allowing you to select from available well groups, or to create a new well group:
- Select 'Create a new well group' and retain the default name.
- Ensure you have the options selected as shown below.
- Click [OK].

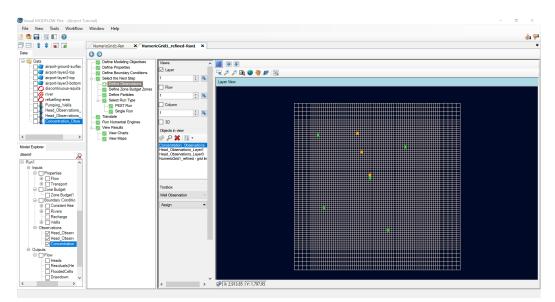
😻 Create/Add Well Observations			\times
Select a Well Observation object from the Data Tree:			
Concentration_Observations			
O Assign observations to an existing well group			
Head_Observations_Layer1			\sim
Assign observations to a new well group			
Concentration_Observations			
	ОК	Can	cel

The observation wells ('Concentration Observations') will be added to the display and the numerical model tree, under **NumericGrid1_refined/Run/Inputs/Observations**.

 Locate 'Concentration Observations', and click on the box beside this data object in the Model Explorer

Model Explorer
Search
🖃 🥘 Conceptual Model1
Model Boundary
🕀 🥘 Structure
Properties
🖃 🚞 Simulation Domain
⊟ Model Domain
Boundary Conditions
NumericGrid1
□ VumericGrid1_refined
⊟ · Run
inputs
III IIII IIIII IIIIIIIIIIIIIIIIIIIIII
⊡ Transport
⊡ ⊡ Zone Budget
□ Zone Budget □ □ □ Boundary Conditions
Constant Heads
⊞ ⊂ Constant riedus ⊞ ⊡ Rivers
techarge ⊕ □ Wells
Head_Observations_Layer1
Head_Observations_Layer3
Concentration_Observations

• You should now see several orange points in the model domain that represent the locations where head measurements were taken.



- Now is a good time to save the project. Click [File]>[Save Project] from the main menu.
- Click [] (Next Step) to proceed.
- Select [Single Run], and click [[(Next Step) to proceed
- At the 'Single Run' step, be sure to include MT3DMS in the engine run; place a check box box beside this engine in the list.
- Click [] (Next Step) to proceed.

MT3DMS Translation Settings

This section will guide you through the selection of the advection method, solver settings, and output times that you will use to obtain the solution and results for the contaminant transport model.

Settings Translation Log DIS	LPF	RIV	CHD	RCH	BAS	OC	PCG	NDC	WEL	IN	
General Settings MODFLOW-2005 Solvers Solvers Recharge and EVT Lake Layers Rewetting Initial Heads Anisotropy Output Control Advanced Settings MT3DMS General Solution Method Output Control Advanced Settings	Min	neral osity Opt urant Nur h. Sat. Th	nber ickness			Effe 0.7 0.0					

Solution Method

• Expand the 'MT3DMS' item under the Translation settings, and select [Solution Method]. A Solution Method settings window will appear.

For this model run you will be using the Upstream Finite Difference solution method with the Implicit GCG Solver. The Upstream Finite Difference method provides a stable solution to the contaminant transport model in a relatively short period of time. The GCG solver uses an implicit approach to solving the finite difference equations, and is usually much faster than the explicit solution method.

- Click the button in the 'Advection Method' option and select [Upstream Finite Difference (UFD)]
- Click the button in the 'Use Implicit GCG Solver' option and select [Yes].

• The Implicit GCG Solver Settings window will appear in the lower half of the translation settings window, as shown in the image below:

Settings Translation Log DIS LPF RIV CHD RCH BAS OC PCG NDC WEL IN
General Settings General Advection Method Upstream Finite Difference (UFD) Use Implicit GCG Solver Yes Solvers Solvers Solvers Solvers Recharge and EVT Lake Layers Arisotropy Output Control Advanced Settings Solvers General Solvers Solvers General Solvers Solvers Arisotropy Output Control General Solvers Solvers Solvers General Solvers Solvers General Solvers General Solver General Solver General Max.number of outer terations I Max.number of inter terations Relative convergence acterion Concentration charge printing interval O O Duption Method General Solver General General General General General General General General Max.number of inter terations I Max.number of inter terations I Max.number of inter terations I General Gene

Although the Upstream Finite Difference method and the Implicit GCG Solver are generally computationally efficient, the tutorial simulation tracks contaminant transport over a 20 year period. In order to speed up the modeling process, you will use a nonlinear time step. Type the following information in the fields at the bottom of the window.

- Maximum transport step size = 200, as in the image above
- Multiplier = 1.1

Output Control Settings

Next, you will define the output times at which you would like to see the contaminant transport modeling results.

- Under the 'MT3DMS' section in the Translation settings, select [Output Control]. The Translation settings will update as shown below.
- Enter 7305 for the 'Simulation time length'
- Enter 5000 for 'Max number of transport steps'
- The remaining defaults can be left as they were found, as shown in the image below:

Settings Translation Log DIS LPF	RIV CHD RCH BAS OC PCG NDC	LMT WEL IN BT3 DP3 RC3 AD3 GC
General Settings General Gene	✓ General Simulation time length (project time units) Max number of transport steps Specify maximum step size Maximum step size (project time units) Save concentation at observation point for every Nth time Save condition at observation point for every Nth time Save CMB/CCM file (mass balance output) Image: Save CMB/CCM file (mass balance output)	7305 5000 No 1 e ste 1

Output Times

- · For this tutorial you will define specified times at which you would like to see the transport simulation results.
- The bottom half of the [Output Control] frame can be used to specify output times
- Click the [44] [Add Row] button; repeat this 7 more times.
- Enter the following output times in the grid.

T	3D Output times
	1
	730
	1460
	2190
	2920
	3650
	5475
	7305

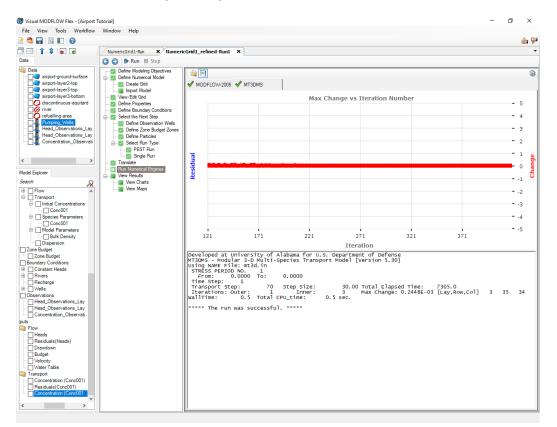
M٦

- Now is a good time to save the project. Click [File]>[Save Project] from the main menu.
- You are now ready to translate the inputs into the MT3DMS packages.
- Click [Translate] to create the MODFLOW-2005 and MT3DMS packages. (this should take approximately 10-20 seconds)
- Click [] (Next Step) to proceed.

Run MODFLOW-2005 and MT3DMS

In this step of the tutorial, you will run the flow and transport model:

- Click the [P Run] button to run MODFLOW-2005 and MT3DMS.
- The MODFLOW model run should complete in a few seconds; the MT3DMS run should also complete in under a minute.
- Once finished, you should see the message "***** The run was successful. ***** at the bottom of the engine progress window.



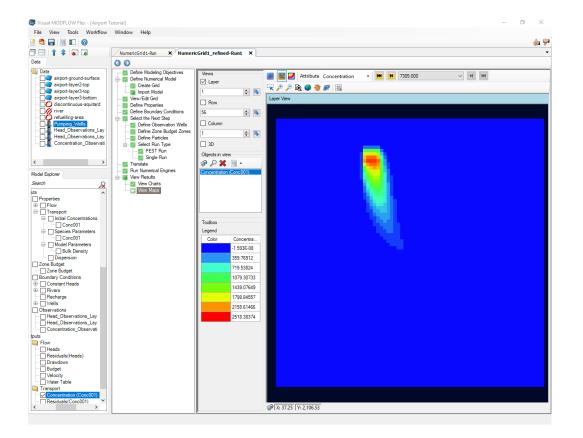
- In addition, you will see several items will be added to the model tree under 'Outputs': the 'Concentrations' was added to the model output tree under 'Output/Transport'.
- Now is a good time to save the project. Click [File]>[Save Project] from the main menu.
- Click [[] (Next Step) to proceed.
- Click [View Maps].

View Maps (Concentrations)

 By default, the Heads will be shown in the Maps view. In order to see the 'Concentrations', you need to turn off 'Heads' from the model explorer and turn on 'Concentrations'.

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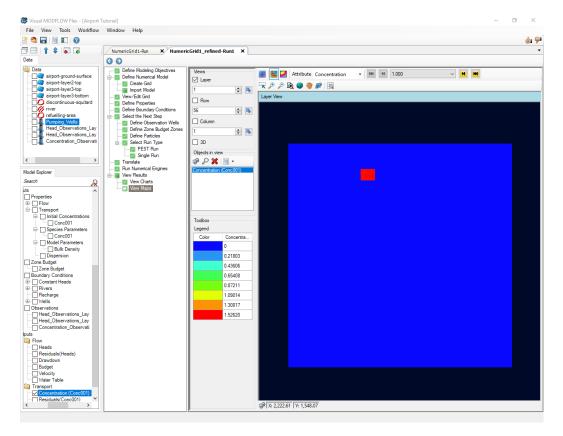
- Locate the 'Output' node on the model tree.
- Remove the Checkbox beside 'Heads'
- Add a checkbox beside 'Concentrations'
- In the viewer toolbar, activate the **'Cells'** rendering option by clicking the **[11]** button and turn off the grid by clicking the **[11]** button:



- The concentration contours will be plotted for the first transport output time (in this case the first transport output time is 1 day).
- In order to see the concentration results at the other output times, you need to advance the output time. Click on the time step buttons located on the toolbar above the 'Layer View', as shown below. Alternately, you can expand the list of output times, and navigate directly to the desired output time.

K	7305.000 ~	H
	1.000 730.000 1460.000 2190.000 2920.000 3650.000 5475.000	
	7305.000	

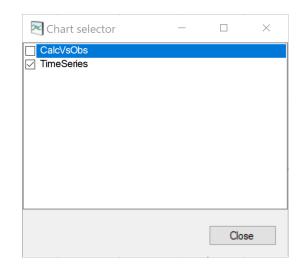
- The display will then update with a plot of concentration contours for the selected output time
- Open the first output time, **1 day**, and the concentrations in the first layer of the model should look similar to the following figure:



View Charts (Concentrations)

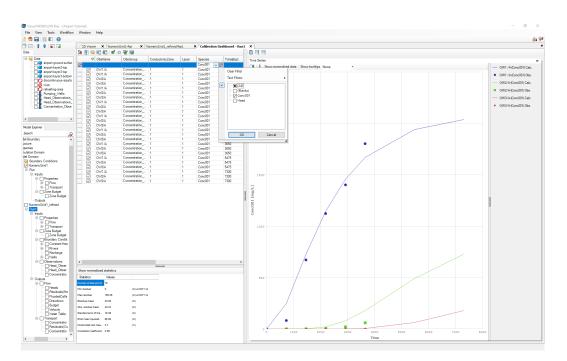
In this section of the tutorial, you will learn how to compare the observed concentration data to the concentration values calculated by the model.

- Select [View Charts] item from the workflow tree.
- Click [Open Dashboard] to proceed.
- Click 'Chart selector' [
- Then, under 'Chart selector' select 'Time Series' and unselect 'CalcVsObs'



- Click [Close]
- Select the dropdown button in the first row of the table for the Species field and click [
 I to select a filter from the Attribute Table. Note, you may wish to expand the table by clicking and dragging the separation line between the table and the chart to the right.
- Deselect all of the checkboxes except "Conc001" and click [OK].

You should now see the breakthrough curves for each of the three concentration observation wells defined earlier in the model (see following figure).



This time-series graph shows the calculated result using a colored line data series while the observation data is displayed only as data point symbols.

 Now is a good time to save the project. Click [File]>[Save Project] from the main menu.

*****This concludes the 'Airport Numerical Model with Transport' tutorial.*****

3.4 SEAWAT Tutorial

The following example walks through creating a simple numerical model with variabledensity groundwater flow (using SEAWAT). The exercise is based on the well-known Elder model.

Objectives

- Learn how to create a project and create a numerical grid for SEAWAT simulations
- Learn how to define new property zones and boundary conditions
- Define inputs/boundary conditions for SEAWAT contaminant transport
- Translate the model inputs into SEAWAT input packages
- Run SEAWAT engines
- Understand the results by interpreting heads, drawdown, and concentrations in several views
- Check the quality of the model by comparing observed heads to calculated heads, and observed vs. calculated concentrations

References

Guo, W., and Langevin, C.D., 2002. User's Guide to SEAWAT: A Computer Program For Simulation of Three-Dimensional Variable-Density Grown-Water Flow. U.S. Geological Survey Open-File Report 01-232. Tallahassee, Florida.

Langevin, C.D., Shoemaker, W.B., and Guo, W. 2003. MODFLOW-2000, the U.S. Geological Survey Modular Ground-Water Model -Documentation of the SEAWAT2000 Version with the Variable-Density Flow Process (VDF) and the Integrated MT3DMS Transport Processes (IMT). U.S. Geological Survey. Tallahassee, Florida.

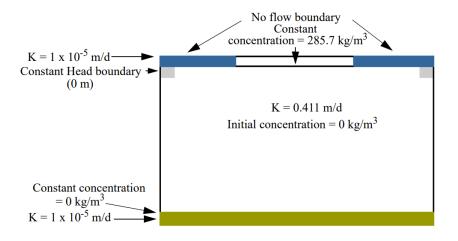
Introduction

Saltwater intrusion is a common occurrence along coastlines throughout the world. Saltwater is denser than freshwater, and consequently will tend to migrate inland underlying freshwater zones when groundwater resources are depleted or in areas where the water table is low. A static equilibrium is reached when the freshwater discharge force balances the buoyancy

force due to density. Visual MODFLOW Flex includes the SEAWAT Engine to simulate saltwater intrusion.

SEAWAT is a computer program for simulating three-dimensional, variable-density, transient ground-water flow in porous media. SEAWAT was designed by combining a modified version of MODFLOW-2000 and MT3DMS into a single computer program. SEAWAT contains all of the processes distributed with MODFLOW-2000 and also includes the Variable-Density Flow Process (as an alternative to the constant-density Ground-Water Flow Process) and the Integrated MT3DMS Transport Process.

This tutorial illustrates a common application for SEAWAT and is based on the Elder Problem published in the User's Guide to SEAWAT (Guo and Langevin, 2002). The basic design of this SEAWAT exercise is shown in the figure below.



The Elder model is commonly used as a benchmark problem for variable-density groundwater flow, where fluid density is a function of salt concentration. This problem simulates salt-water intrusion and proliferation through a freshwater aquifer. Molecular diffusion is the sole mechanism of hydrodynamic dispersion during the simulation, which runs for 20 years. Salt from the constant-concentration boundary at the top of the model diffuses into the model domain and initiates a series of complex vortices that redistribute the salt mass throughout the model. A constant-concentration boundary with a value of zero is specified for the lowest layer in the model. Two outlet cells with constant head values of zero are specified for the upper left and right boundaries. These constant head cells allow salt to diffuse into the model by providing an outlet for fluid and salt mass (Guo and Langevin, 2002).

Create the Project

- Launch Visual MODFLOW Flex.
- Select [File] then [New Project..]. The Create Project dialog will appear.
- Type in project name 'SEAWAT_Elder'.
- Click the [^[]] button, and navigate to a folder where you wish your projects to be saved, and click **[OK]**.
- Define your coordinate system and datum (or just leave the Local Cartesian as defaults).

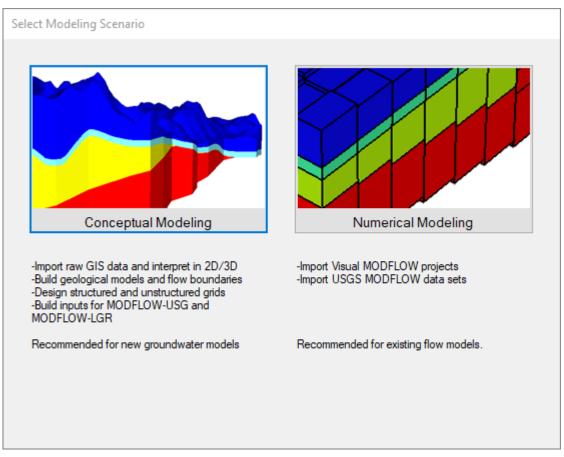
- Most of the default units will be fine, but we will need to update the conductivity units.
- Select [m/d] as the Conductivity units
- Click **[OK]** button in the lower right corner of this window.

• Note: It is recommended to select the folder "C:\Users\User_Name\Documents\VMODFlex" as the default location for your projects. You may then add a new folder to each individual modeling project. For the purposes of this project you may create the sub-folder SEAWAT_Elder. A new folder can be created automatically by selecting the 'Create a folder for the project' button under Data Repository.

Before clicking OK, the Create Project dialog should look like the image below:

🕽 Create Project	? ×
Project Information	Units *
Name: *	
SEAWAT_Elder	✓ Unit Settings
	Concentration mg/L
Data Repository: *	Conductivity m/d
C:\Visual MODFLOW Flex	Density (includes Bulk De kg/m^3
	Groundwater Flow m^3/d
Create a folder for the project	Length m
Description:	Mass kg
	Mass Flow mg/yr
	Pumping Rate m^3/d
	Recharge mm/yr
	Specific Storage 1/m
	Stream Flow m^3/d
	Temperature °C
	Time day
Project Coordinate	Volumetric Flow m^3/d
Coordinate Systems: *	
Local Cartesian v	
Datum: *	Conductivity
World Geodetic System 1984	
	OK Cancel Help

The following window will then appear:



The Select Modeling Scenario allows you to choose whether to proceed with the Conceptual or Numerical modeling workflow. The conceptual modeling workflow allows you to import data objects into Visual MODFLOW Flex and to build a conceptual site model (CSM) that is grid independent. The CSM can then be used as a starting point for several different numerical models. In other words, numerical models (i.e. with different grid types, engines, etc.) can be quickly and easily created based on the same conceptual model. This makes it easy for you to manage several different numerical models with slight variations.

Conceptual modeling is not covered in this exercise, so we will proceed with the numerical modeling workflow

• Select [Numerical Modeling] and the Numerical Modeling workflow will load.

Proceeding with the numerical modeling workflow will bring you to the first step in the that workflow, which is to define your model objectives. This step allows you to specify whether you will be running a fully saturated or variably saturated model, whether it will be a constant or variable density model, whether contaminant transport will be included, which flow/transport engines will be utilized, etc.

The selection of these modeling objectives will determine which model- and species-specific transport properties must be defined (e.g. molecular diffusion coefficients, distribution coefficients, decay constants, etc.). It is also possible to define default property values at this time.

For the default project properties please input the values as shown figure below.

- Select Flow type: Saturated (Variable Density)
- Select Simulation type: Groundwater flow
- Available Flow Engines: USGS SEAWAT from WH
- Select Start Date: today
- Type: Kx (m/d) = 0.411 in the Default Project Property Settings frame
- Type: Ky (m/d) = 0.411 in the Default Project Property Settings frame
- Type: Kz (m/d) = 0.411 in the Default Project Property Settings frame
- Type: Initial Head = 1E-6 in the Default Project Property Settings frame
- Type: Ss (1/m) = 1E-05 in the Default Project Property Settings frame
- Type: Sy = 0.1 in the Default Project Property Settings frame
- Type: Name = Salt in the Species Parameters table
- Type: Description = Salt in the Species Parameters table
- Type: DRHODC = 0.7 in the Species Parameters table
- Type: MDCOEFF = 0.308 in the Species Parameters table

• **Note**: MDCOEFF is the species-specific molecular diffusion coefficient. This parameter is only used if the multi-diffusion option is set to true in the DSP package advanced settings. While we have entered a value here, it will not be used. We will specify a model-wide molecular diffusion coefficient at a later step.

🐯 Visual MODFLOW Flex - [SEAWA	\T_Elder]											-		
Eile View Jools Workflow	<u>W</u> indow <u>H</u> elp													
2 🍕 🔚 🔢 🗈 🛛													<u>ا</u> ھ	
3 🗆 🛊 🛊 📭 😱 🦳	Numerical Model ×													
Data	00													
Node Expore Sourch &	Constant income income income in the interval income income in the interval income interval income in the interval income interval income in the interval income interval interv	Stat Date Saturday , January 1.	2000 	No sorption simu Reaction No kinetic reactiv Available Transpor	lated Description Sat	Note 2	Teperdue	Initial concentration 0	CREF 0	Uvis ingrit	07 07	DMUCC m 20eg) 0		

Now that the modeling objectives are defined you may advance to the next step of creating the numerical grid. Click the white right arrow in the blue circle at the top of the Numerical Model window to advance to the Define Numerical Model step.

- Click [[(Next Step) to proceed to the Define Numerical Model workflow step
- Click [Yes] to dismiss the warning message about the model start date

• Now click on the [Create Grid] icon

Define Model Grid

We will now proceed with the model grid creation. You should now see the **Create Grid** workflow step, as shown in the image below:

We will create a grid with 1 row, 44 columns and 27 layers. Specifying the number of rows/columns and the overall grid extents horizontally will be quite easy, as these values can be specified directly in this window. To specify layer elevations for all 27 layers would be quite tedious though, so we will initially create the grid with a single layer with the elevations being the maximum and minimum final layer elevations. We will then refine the initial layer into 27 equally thick layers.

Please input the number of Rows and Columns and change the number of layers to 1. The top elevation of the first layer shall be set to 6 m, and the bottom elevation to -156 m.

- Rows = 1 in the Grid Size frame
- Columns = 44 in the Grid Size frame
- X Min = 0 in the Grid Extents frame
- X Max = 600 in the Grid Extents frame
- Y Min = 0 in the Grid Extents frame
- Y Max = 13.636 in the Grid Extents frame
- **Cell width = calculated** this value can be adjusted as per project requirements
- Cell height = calculated this value can be adjusted as per project requirements

- Number of Layers = 1
- Layer1 Top Elevation = 6
- Layer1 Bottom Elevation = -156

The screen should now look like the image below:

• [Create Grid] button at the top-left of preview window

The **Model Explorer** (the lower left section of the interface) will be populated with the newly created model structure items. You will also see 2 new surfaces created in the Data Tree. These surfaces represent the top and bottom surfaces of the model layers and are consequently transformed automatically into 'Horizons' in the Model Explorer. Each pair of horizons in turn defines a zone, so you will also notice one new zone in the Model Explorer.

Your grid has been created and you'll notice that the Properties section of the model structure is empty, so the next step will be to define boundary conditions and the model properties. The '**View/Edit Grid**' portion of the workflow allows the user to make any necessary changes to the grid structure. This will be particularly useful for us, since we need to refine our initial grid vertically to have 27 layers (as defined by the original Elder model).

Click [[(Next Step) to proceed to the View/Edit Grid step

In the middle of the interface you will see a **Toolbox**. The buttons under this toolbox allow you to edit the grid in the horizontal direction (i.e. **Edit Grid...**), to edit the grid in the vertical direction (i.e. **Edit layers...**), to extract a subgrid from your model (i.e. **Create subgrid...**), or

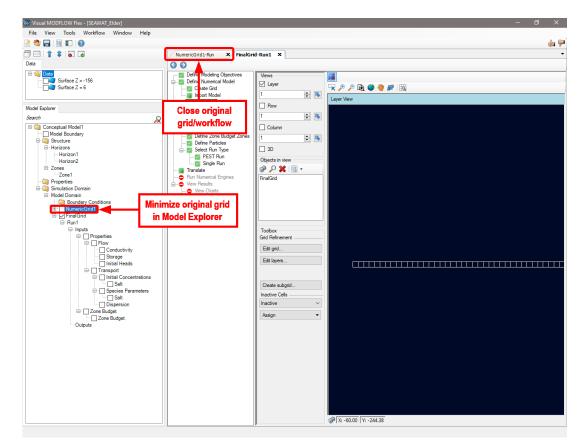
to assign model cells as active/inactive (i.e. the **Inactive Cells** frame). We will utilize the **Edit layers** functionality to refine our initial single layer grid, and then use the **Inactive Cells** feature to deactivate several flow cells in the top model layer.

- Click the [Edit layers...] button under the Toolbox
- Type: FinalGrid in the New grid name field
- Type: 27 in the By a factor of field
- Click the [Apply edit] button at the bottom left
- The window should look like the following:

Edit layers	- 🗆 X
Layer edit details Script	
New grid name	
FinalGrid	Viewing Row 🔹 1 🚖 Exaggeration 2 🚖 🔎 🔎 🌘 🍓
Overwrite existing grid	
Refine Insert Remove Replace From layer	
	Layer: 26 Row: 1 Column: 2 X: 27.14 Z: -147.14
Apply edit Undo edit Reset	Add objects using the Data and Model Explorer tree checkboxes
	OK Cancel Help

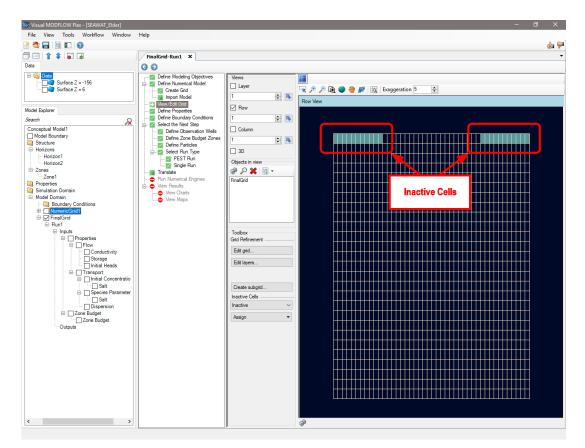
• Finalize the layer edit by clicking [OK]

Once again you should see that the **Model Explorer** will be populated with the newly created model structure items, and a new workflow window will open. We will continue working with the **FinalGrid** workflow, so feel free to minimize the initial grid in the Model Explorer, and close the initial workflow window:



The final change to the grid is to specify two inactive areas in model layer #1. To make this change we will activate the **Row** view (Row 1) and assign inactive cells using the polyline drawing function:

- **I** Row in the Views frame, to activate Row view
- Layer in the Views frame, to deactivate Layer view
- Exaggeration: 5 in the field above the viewer to decrease the vertical exaggeration
- [Assign] > [Using Polyline] button under the Toolbox, under Inactive Cells
- Draw a polyline in layer 1, from Column 1 to 11 (click once to start, double-click to finish)
- Draw another polyline in layer 1, from Column 34 to 44 (click once to start, double-click to finish)
- [Finish] button under the Toolbox
- [OK] in the Copy to Row(s) window that appears
- The final grid should look like the image below:



We have now recreated the grid as required by the Elder model and are ready to proceed to the next step in the workflow, which is to define property values.

Click [(Next Step) to proceed to the Define Properties step

Define Properties

You should now be viewing the **Define Properties** workflow step. You may want to inspect that the model properties are set according to the default property values that you defined during the Define Modeling Objectives step. Select any of the properties from the toolbox and click on the **Edit...** button, and you will see the values assigned to each cell of the model for the respective property. For example, the image below displays the Edit Property window for the conductivity property group:

• Click [Edit...] in the Toolbox to open the Edit property window for a given property group

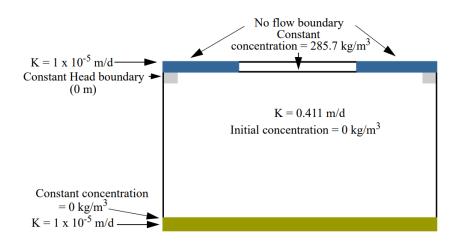
it Cells Script	T					
ones	Conductivity	Calculation	√:	π 📰 📰		
Zone	Layer	Row	Column Y	❤ Kx (m/d)	❤ Ky (m/d)	マ Kz (m/d) マ
1	▶ 1	1	12	0.411	0.411	0.411
	1	1	13	0.411	0.411	0.411
	1	1	14	0.411	0.411	0.411
	1	1	15	0.411	0.411	0.411
	1	1	16	0.411	0.411	0.411
	1	1	17	0.411	0.411	0.411
	1	1	18	0.411	0.411	0.411
	1	1	19	0.411	0.411	0.411
	1	1	20	0.411	0.411	0.411
	1	1	21	0.411	0.411	0.411
	1	1	22	0.411	0.411	0.411
	1	1	23	0.411	0.411	0.411
	1	1	24	0.411	0.411	0.411
	1	1	25	0.411	0.411	0.411
	1	1	26	0.411	0.411	0.411
	1	1	27	0.411	0.411	0.411
	1	1	28	0.411	0.411	0.411

• Click [OK] in the dismiss the Edit property window

Remember that at any step during the numerical workflow you have the possibility to inspect your grid in four different views: plan, two cross-section views and a 3D view. These views can be toggled on and off by checking the respective check-boxes in the **Views** area. Make sure you are looking at Row 1 in the Layer View window. If you have more viewer windows open, make sure that Row View is the active window, as shown in the image below:

Views	
Layer	🖳 🔎 🔎 🗟 🌒 🚛
1 😫 隊	Row View
Row	Now view
1	
Column	
1 💺 隊	
□ 3D	

Now we will assign property values as shown in the following image:



We will begin with the conductivity values for the top and bottom model layers:

- Select [Conductivity] from the first menu in the Toolbox frame
- Click [Assign] > [Polyline] buttons under the Toolbox
- **Type: 5** in the **[Exaggeration]** field above the viewer to decrease the vertical exaggeration
- Draw a polyline across all of layer 1 (click once to start, double-click to finish)
- Draw another polyline across all of layer 27 (click once to start, double-click to finish)
- Click [Finish] button under the Toolbox
- The New Property Zone window will open.

In this window we will assign the selected cells to a **New** property zone, and apply the desired Kx, Ky and Kz values (i.e. 1E-05 m/day).

- [New] button at the top-left of the window, to create a new property zone
- Type: 1E-05 in the Value field for Kx, Ky and Kz
- [OK] to accept inputs and create the new property zone
- The **New Property Zone** window should look like the image below before clicking **[OK]**:

New F	Property Zone													
Zone 2		New								Assign		Rows		
Zone	Attributes	11.0								1	*			
<u> </u>	Parameter	Unit	Method		Value	-	Object	•	Napping	To Row				
	Kx	m/d	Constant	~		•			~	1	-			
	Ку	m/d	Constant	\sim	1E-05	$\mathbf{\mathbf{x}}$			~					
+	Kz	m/d	Constant	\sim	1E-05	₩			~					
												ОК	Can	cel

We will repeat this process for initial concentrations, assigning a value of **285,700 mg/L for layer 1 ONLY**.

- Select [Initial Concentration Salt] from the first menu in the Toolbox frame
- Click [Assign] > [Polyline] buttons under the Toolbox
- Draw a polyline across all of layer 1 (click once to start, double-click to finish)
- Click [Finish] button under the Toolbox
- The New Property Zone window will open
- Click the [New] button at the top-left of the window, to create a new property zone
- Type: 285700 in the Value field for Concentration
- [OK] to accept inputs and create the new property zone

The remaining changes to property values will be made to the entire model, so we can use the **Edit** function rather than assigning new property zones using the drawing tools. We will update the effective and total porosity values (through the **Storage** property group) and longitudinal dispersivity (through the **Dispersion** property group).

- Select [Storage] from the first menu in the Toolbox frame
- Click [Edit...] button under the Toolbox
- Type: 0.1 in the Effective Porosity column, then use [F2] to propagate through all cells
- Type: 0.1 in the Total Porosity column, then use [F2] to propagate through all cells
- [OK] to accept inputs and create the new property zone
- Select [Dispersion] from the first menu in the Toolbox frame
- Click [Edit...] button under the Toolbox
- Type: 0 in the Longitudinal dispersivity (m) column, then use [F2] to propagate through all cells
- [OK] to accept inputs and create the new property zone

Finally, one final change must be made to the model level dispersion parameters. These can be accessed by right-clicking the **Dispersion** property group under the **Model Explorer** and selecting **Dispersion Parameters** as shown in the image below:

- Right-click **Dispersion** from the **Model Explorer** (under FinalGrid1 > Run1 > Inputs > Properties > Transport)
- Click [Dispersion Parameters] from the menu that appears

FinalGrid Fun1 Properties Flow Flow Conductiv Storage Initial Hea Transport Initial Con Salt Dispersio	ds centratio arameter		× •
Zone Budget	Flex Viewer	Color Zone	
Outputs	Rename	1	
	Delete		
	Edit Property Zones		
	Settings		
	Export		
	Dispersion Parameters		
	3D Viewer		
	Expand to selection		
	Expand all child nodes		
	Collapse all		
<	>		

- The Dispersion Parameters window will open
- Type: 0.308 in the Diffusion Coeff. (m^2/day) field, then use [F2] to propagate through all cells
- Click [OK] to confirm and assign values

	Layer	Horiz/Long Dispersivity	Verti/Long Dispersivity	Diffusion Coeff. (m^2 / day)	
•	1	0.1	0.01	0.308	
	2	0.1	0.01	0.308	
	3	0.1	0.01	0.308	
	4	0.1	0.01	0.308	
	5	0.1	0.01	0.308	
	6	0.1	0.01	0.308	
	7	0.1	0.01	0.308	
	8	0.1	0.01	0.308	
	9	0.1	0.01	0.308	
	10	0.1	0.01	0.308	
	11	0.1	0.01	0.308	

• **Note**: this diffusion coefficient is the modelwide molecular diffusion coefficient. This is different than the species-specific diffusion coefficient applied during the Define Modeling Objectives step. The species-specific value is only used if the multi-diffusion option is set to true in the DSP package advanced translation settings.

Now is a good time to save the project.

• Click [File] > [Save Project] from the main menu

Define Boundary Conditions

If you are satisfied with the property values assigned to the model, advance to the **Define Boundary Conditions** step in the numerical workflow. We will assign the model boundaries in Row view.

• Click [[(Next Step) to proceed to the Define Boundary Conditions step

At this stage we will assign boundary conditions to our model, starting with a constant head boundaries at the top-left and top-right corners of the model (see the figure at the very beginning of this tutorial). We will do this by simply selecting the two desired cells.

- [Constant Head] from the first menu under the Toolbox
- [Assign] > [Cells] from the menu under the Toolbox
- Left-click once in Layer 2, Row 1, Column 1
- Left-click once in Layer 2, Row 1, Column 44
- Click [Finish] under the Toolbox
- The Define Boundary Condition window will open

• Click [Next>>] to accept default name and proceed

We will assign a constant head value of 0 m to both of the selected cells. For both cells, type a value of 0 in the starting and ending head fields, select **Specified Density** as the density option, and apply a density of 1000 kg/m³.

- Type: 1E-6 in the Starting Head (m) field, for both cells/rows
- Type: 1E-6 in the Ending Head (m) field, for both cells/rows
- Select Specified Density in the Density Option field, for both cells/rows
- Type: 1000 in the Density (kg/m^3) field, for both cells/rows

Schedule Static •	 Name Cor	nstant Head	11	🤹 Ca	Iculation 1000	√3	x 😐 🔳 💷		
This boundary condition is static.	Layer *	Row T	Colu 🛛	Starting Hea 🛛	Ending Hea 🔻	Density Opt 🕁	Density (kg/ 🕁	Salt (m 🔻	Activ N
transient to deline a schedule.	▶ 2	1	1	1E-06		Simulated de		-1	\checkmark
	2	1	44	1E-06	1E-06	Simulated de	1000	-1	\checkmark

• Click the [Finish] button to finalize and create the constant head boundary condition

You will notice that both of the selected cells will be populated with red dots. These red dots represent the newly created boundary condition. Boundary conditions within Visual MODFLOW Flex are color-coded for quick identification.

We will now apply two constant concentration boundary conditions. In the top layer we will apply a high salt concentration (285.7 kg/m³), and in the bottom layer we will apply a constant concentration of 0 kg/m³. This concentration gradient is what will drive water flow and solute transport in this model.

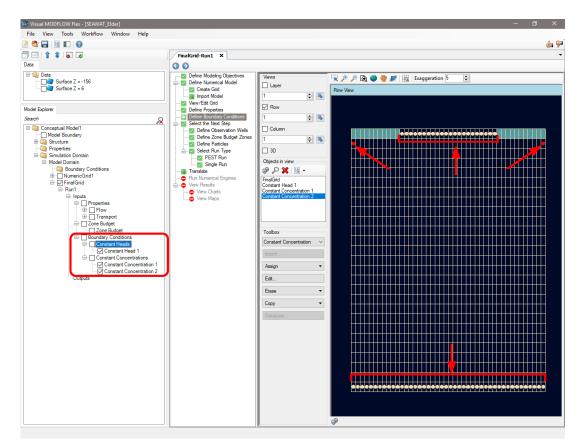
- [Constant Concentration] from the first menu under the Toolbox
- [Assign] > [Polyline] from the menu under the Toolbox
- Draw a polyline across active zone of layer 1 (click once to start, double-click to finish)
- Click [Finish] under the Toolbox
- The Define Boundary Condition window will open
- Click [Next>>] to accept default name and proceed
- Type: 285700 in the Salt (mg/L) field, then use [F2] to propagate through all cells
- Click the [Finish] button to finalize and create the constant head boundary condition

• Note: if the drawn polyline extends into the inactive zone, you may see a **Resolve validation** failures window appear. In this case it is simply identifying that some of the selected cells are in the inactive zone, and the boundary conditions for those cells can either be deleted or the cells can be reactivated. The default solution will be to **Delete invalid cells**. If you DO see this window, simply click **Apply** then **Close** to resolve potential validation errors.

Now we will repeat the steps above to apply a constant concentration of 0 mg/L to the lowest model layer.

- [Constant Concentration] from the first menu under the Toolbox
- [Assign] > [Polyline] from the menu under the Toolbox
- Draw a polyline across active zone of layer 27 (click once to start, double-click to finish)
- Click [Finish] under the Toolbox
- The Define Boundary Condition window will open
- Click [Next>>] to accept default name and proceed
- Type: 0 in the Salt (mg/L) field, then use [F2] to propagate through all cells
- Click the [Finish] button to finalize and create the constant head boundary condition

Now all of the desired boundary conditions have been applied across the entire model domain. Your display should look something like the image below. Note the beige dots in layers 1 and 27, indicating the presence of the constant concentration boundaries. Also note the red dots indicating the constant head boundaries in layer 2 (top-left and top-right). Finally, note how each new boundary condition has been added into the **Model Explorer**.



We now have enough data to run this density-driven flow model, but first we have to define our model translation settings.

Translate and Run the SEAWAT Model

Navigate to the **Select Run Type > Single Run** step in the numerical workflow. You may click directly on this step as it is colored green, or you can navigate there step-by-step using the navigation arrows at the top of the workflow window.

 Click [Single Run] from the Workflow Navigator, to proceed directly to the Single Run workflow step

You will be prompted to select which engines to run. By default, **USGS SEAWAT from WH** should already be selected. This is because this is the only flow engine within Visual MODFLOW Flex that allows you to model density-dependent flow. If you click on the Flow Engine menu you will see that USGS SEAWAT from WH is the only available option. The engine settings should look like the image below:

Flow Engine		
USGS SEAWAT from WH	\sim	
🗹 Run Transport Engine		
USGS SEAWAT from WH	~	
ZONEBUDGET		
Particle Tracking		
	\sim	1

You will now advance to the **Translate** step of the workflow. This step will translate all the input data defined for the model into "packages" (i.e. text files) that can be run by SEAWAT.

• Click [[] (Next Step) to proceed to the Translate step

The translation settings will appear; this allows you to adjust solvers and their parameters (number of iterations, head-change criterion, damping factors), package settings, output control, etc.. In the **Settings** section of the **SEAWAT** branch you can change the **Steady-State Simulation Time** to 7300 by entering this value directly.

- Go to the [SEAWAT] > [Settings] section of the menu
- Select BCF6 in the Property Package field.
- Dismiss the warning about the VSC package which will be turned off later
- Type: 7300 in the Steady-State Simulation Time field
- Select Transient in the Run Type field
- Type: 20 in the Time Steps field
- Type: 1 in the Multiplier field
- Go to the [SEAWAT] > [Solvers] section of the menu
- Select Conjugate Gradient Solver (PCG) in the Selected Solver field
- Type: 50 in the Max. Outer Iterations (MXITER) field
- Type: 25 in the Max. Inner Iterations (ITER1) field
- Type: 1.0E-7 in the Head Change Criterion (HCLOSE) field
- Type: 1 in the Residual Criterion (RCLOSE) field
- Type: 5 in the Printout Interval (IPRPCG) field
- Go to the [SEAWAT] > [Layers] section of the menu
- Apply layer type '0: Confined, constant S,T' for ALL layers
- Go to the [SEAWAT Transport] > [General] section of the menu
- Select Total in the Porosity Options field
- Type: 0.1 in the Courant Number field
- Type: 0.05 in the Min. Sat. Thickness field

- Go to the [SEAWAT Transport] > [Solution Method] section of the menu
- Select Central Finite Difference (CFD) in the Advection Method field
- Select Yes in the Use Implicit GCG Solver field
- Type: 1E-08 in the Relative Convergence Criterion field
- Type: 5 in the Concentration change printing interval field
- Select Modified Incomplete Cholesky in the Preconditioners field
- Type: 30 in the Initial step size (DT0) (days) field
- Type: 0 in the Max step size (days) field
- Go to the [SEAWAT Transport] > [Output Control] section of the menu
- Type: 7300 in the Simulation time length (project time units) field
- Type: 3000 in the Max number of transport steps field
- Click [Add row] x6 press the Add row button six times to specify six output times
- **Type: 365** [press Tab], **730** [press Tab], **1095** [press Tab], **3650** [press Tab], **5475** [press Tab] and **7300** as the desired output times in each row

The solver settings window for the **Output Control** section should look like the image below:

General	✓ General		
Settings	Simulation time length (project time units)	7300	
. SEAWAT	Max number of transport steps	3000	
···· Settings	Specify maximum step size	No	
Solvers	Maximum step size (project time units)	1	
···· Recharge and EVT	Save concentation at observation point for every N	th time ste 1	
Lake	Save one-line summary of mass budget for every N	h time ste 1	
Layers	Save CMB/CCM file (mass balance output)	Yes	
Rewetting			
Initial Heads			
Anisotropy			
Output Control			
Advanced Settings			
SEAWAT Transport			
- Output Control	₩		
⊕ Advanced Settings		Time	
	365		
	730		
	1095		
	3650		
	5475		
	7300		

It is also important to know that individual settings for the SEAWAT variable-density flow (VDF) and viscosity (VSC) packages can be set through the **SEAWAT Transport > Advanced Settings** menu.

The VDF translation menu allow you to specify how groundwater densities are calculated using the **Density Option** setting (i.e. using salt only, using multiple species, or using user-specified densities), how internodal density is calculated (i.e. central-in-space or upstream-weighted algorithm), whether a variable density water table correction is applied or not, and to specify constants such as minimum/maximum fluid density, and a reference fluid density.

• Go to the [SEAWAT Transport] > [Advanced Settings] > [VDF] section of the menu

- Select Up-stream weighted algorithm in the Intermodal density calculation algorithm field
- Select Not applied in the Variable density water table correction field
- Type: 0.001 in the Initial Time Step field
- Select the Explicit coupling using one iteration option

Settings								
<u> </u>	~	General						
Settings		CUnit		57				
📥 SEAWAT		Ext		.VDF				
Settings		LUnit		67				
Solvers		Run		Yes				
Recharge and EVT		Translate		Yes				
Lake	~	VDF						
Layers		Density option		Calculate density from salt only				
Rewetting		Internodal density calculation algorithm		Up-stream weighted algorithm				
Initial Heads		Variable density water table correction		Not applied				
Anisotropy		Initial time step		0.001				
Output Control								
SEAWAT Transport								
General								
Solution Method								
Output Control		Implicit coupling using DNSCRIT						
Advanced Settings								
ADV		Explicit coupling with one iteration						
BTN		Explicit coupling with multiple iterations						
DSP	-							
GCG			umber of implicitly coupling iterations for VDF and IMT					
LMT		20 🗘						
RCT								
SSM	Mir	nimum Fluid Density	Maximum Flu	uid Density				
VDF	0	↓ kg/m^3	0	↓ kg/m^3				
I VSC		housed						
	Re	ference Fluid Density						
	10	100 🚖 kg/m^3						
		[10004]						
	Elu	id density convergence criterion						
		0001 ¢ kg/m^3						
		v Kg/ii S						

The VSC translation settings allow you to specify how groundwater viscosities will be calculated in the simulation. The **Viscosity Option** setting allows you to choose whether viscosity is calculated using salt only (no temperature dependence), using temperature and additional species (e.g. salt), or whether specifies viscosities will be used. You can also specify constant values such as maximum, minimum and reference viscosities in this menu. If you access the VSC translation settings menu you should see the following:

Settings		
	General	
Settings	CUnit 65	
🖕 SEAWAT	Ext .VSC	
Settings	LUnit 75	
Solvers	Run Yes	
Recharge and EVT	Translate Yes	
Lake	VSC	
Layers	Viscosity option Calculate viscosity from salt	t only - no temperature depend
Rewetting		
Initial Heads		
Anisotropy		
Output Control		
Advanced Settings		
E SEAWAT Transport		
General		
Solution Method	Hartman Marana	
Output Control	Minimum Viscosity Maximum Viscosity	
Advanced Settings	0 🚖 kg/m/day 0 🚖 kg/m/day	
BTN	Reference Viscosity	
DSP	0.000894 \$ kg/m/day	
GCG	v.00034	
BCT		
SSM		
- VDF		
VSC		

However, we do not actually want to run the .VSC package in this simulation, assuming that there is no viscosity effects at higher concentrations. To remove the .VSC package from this model we will change both the 'Run' and 'Translate' fields to 'No'.

- Select [No] in the Run field
- Select [No] in the Translate field

At this time the desired translation settings have all been specified and we can proceed to translating the model input files. Press the translate button to begin the translation process. As soon as you click the translate button Visual MODLFOW Flex will begin translating all the required input files for a SEAWAT model.

- Click [Translate] to create the SEAWAT input packages. Check the log to confirm the translation has finished.
- Click **[Yes]** to dismiss the warning about initial heads

A translation log will run for a few moments and should terminate with the following message:

You should also see a series of new tabs at the top of the translation window, corresponding to the various input files which have been generated. You can click these tabs to view the

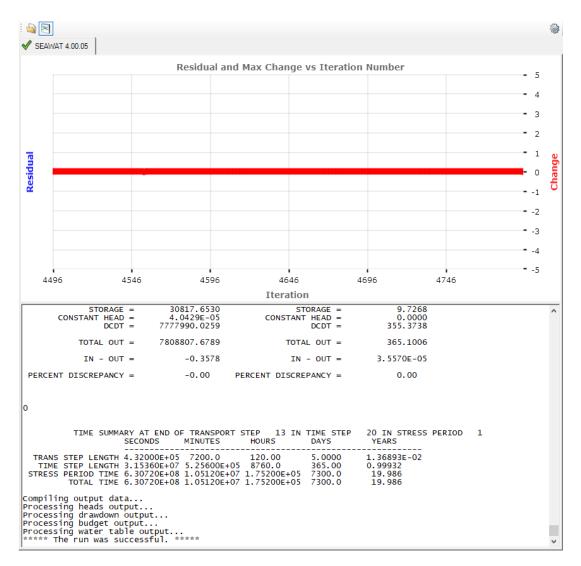
contents of each input file. You can also click the open file button [1991] to open the folder containing the input files. If you aren't happy with the translated files you can always return to the Settings tab, make changes and retranslate the files. For this model run you won't need to make any further changes.

🔌 🗖																	
Settings	Translation Log	DIS	LPF	BAS	OC	PCG	LMT	VDF	CHD	BT3	AD3	DP3	RC3	GCG	SS3	IN	
4:25:42 4:25:42 4:25:42 4:25:42 4:25:42	PM DSP Package	translat complet started	or: Finaliz ed: 'Conc	ze ceptual M		03'											^

You may now proceed to the Run Numerical Engines step.

Click [] (Next Step) to proceed to the Run step
Click [Run] to run the SEAWAT model

The numeric engines will start running and display progress in the main window. SEAWAT will run first followed by any secondary engines selected during the **Single Run** workflow step (e.g. MODPATH or ZoneBudget; we haven't selected any additional engines in this model). Each engine will have an information window that displays simulation results and progress. Clicking on the tab of the respective window will enable you to view detailed results of each run. When your model is finished running your results screen should look like the image below:



If you would like to inspect a record of the run process you may open the listing (.LST) file by

clicking on the **Open Engine Files...** button [^[]] at the top of the window. The model run may take several minutes to complete, since SEAWAT models are more complex than most contaminant transport models. A SEAWAT model may take 2-4 times longer to run than a MODFLOW model of the same dimensions due to the coupling of flow and transport processes.

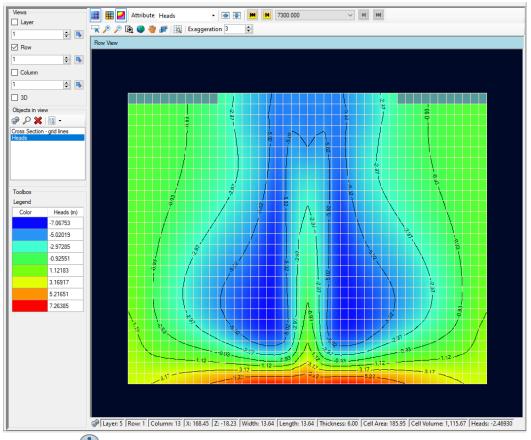
Output Visualization

To see the results of the simulation navigate to **View Results -> View Maps** in the workflow tree. Equipotentials will be shown in plan view by default. You may want to change your map appearance by using the icons at the top of the window and/or right clicking on Heads in the **Model Explorer** and select **Settings...**. To see your equipotentials and the water table in cross-section activate the **Row** viewer (put a check-mark) and select the row number along which you would like to inspect the results.

• Click [[(Next Step) to proceed to the View Results step

- Click [View Maps] to proceed to the View Maps workflow step
- Layer in the Views frame, to deactivate Layer view

Depending on your settings, you should see something like the figure below:

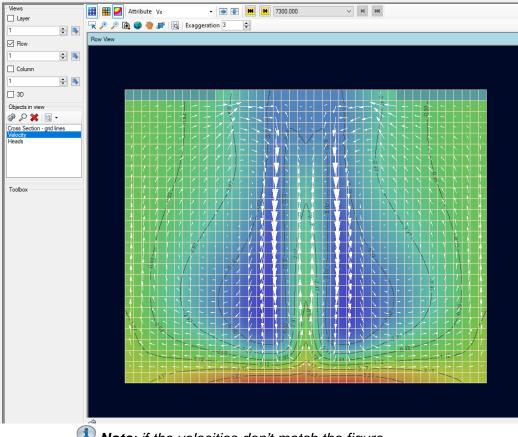


Note: you can maximize the viewer window by deactivating the Model Explorer and/or Workflow

Navigator panels. Use the toolbar buttons I^{\blacksquare} I to turn these panels on/off.

To better visualize the flow field in the model domain you can activate the **Velocity** outputs under the Model Explorer. The velocity flow field indicates that the diffusive flux of salt in the model domain is driving water flow in two recirculation cells, with the greatest flow velocities in the middle of the model and circulating upward toward the edge of the model where the constant heads boundaries have been applied.

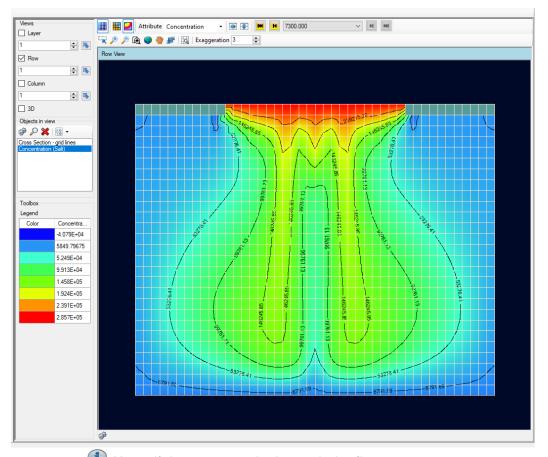
Activate ☑ Velocity under the Outputs/Flow section of the Model Explorer



• **Note**: if the velocities don't match the figure above initially, try toggling the velocities and/or selecting 7300 from the time control bar in the toolbar.

Now you may activate the concentration results, which will display the diffusion of salt throughout the model domain at different output times:

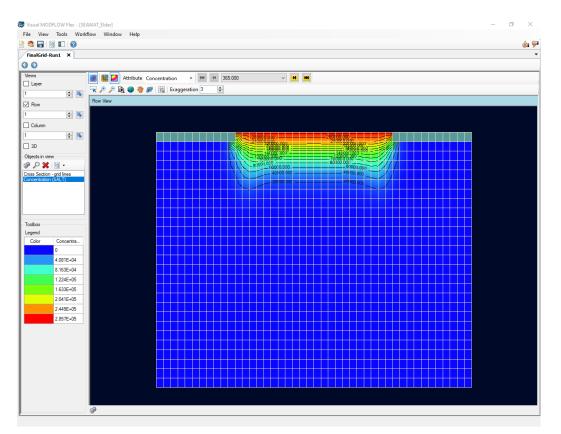
- Deactivate I Heads under the Outputs/Flow section of the Model Explorer
- Deactivate I Velocity under the Outputs/Flow section of the Model Explorer
- Activate I Concentration (Salt) under the Outputs/Flow section of the Model Explorer
- Press the last time step button [III] in the time controls



• **Note**: if the contours don't match the figure above initially try right-clicking 'Concentration (Salt)' from the Model Explorer, accessing the contour line settings and updating the minimum contour level to 0 mg/L.

You can use the time-step picker buttons above the Flex viewer to display the concentration results at various output times. If you update the viewer to display the results at day 365 you should see something like the image below:

• Press [^{IIII}] under the Outputs/Flow section of the **Model Explorer**



Using the cell-inspector tool, review salt concentrations throughout model layer 2 and you should notice some unusual results.

• Press [I under the Outputs/Flow section of the Model Explorer

The **Cell Inspector** window will open, allowing you to select which information will be displayed on a cell-by-cell basis. We're only interested in the results of the model run, so we can deactivate the position, properties, and boundary conditions categories:

- **D Position** to turn off position information
- Properties to turn off properties information
- Boundary Conditions to turn off boundary condition information
- Budget turn off the flow budget information
- Click once on Layer 2, Row 1, Column 11

The **Cell Inspector** window will now display the results of the simulation for the selected cell, as shown in the image below. You can see from these cell inspector results that the salt concentration in cell 2, 1, 11 is **-43,772 mg/L**. These results clearly include non-physical values (e.g. negative concentrations) and can be attributed to truncation errors and/or numerical dispersion associated with the selected solution method for the transport equation (i.e. Central Finite Difference method).

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	Vy	0.0000e+000	m/day
	Vz	2.0398e-002	m/day
	V	1.2814e-001	m/day
	DVx	1.2651e-002	m/day
	DVy	0.0000e+000	m/day
	DVz	2.0398e-003	m/day
	DV	1.2814e-002	m/day
🖃 Co	ncentration (Salt)		
	Concentration	-43772.11761474	mg/L

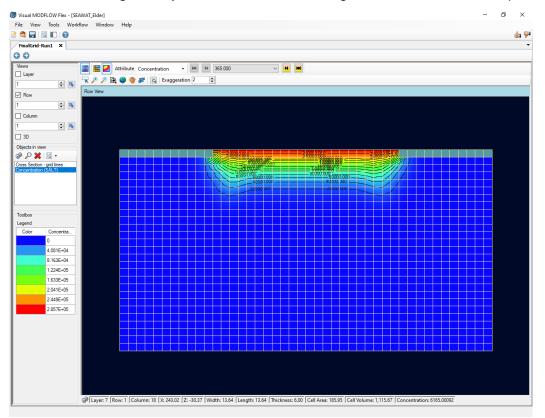
You can improve the results by adjusting the solution method inputs. Return to the **Translate** workflow step and make the following changes:

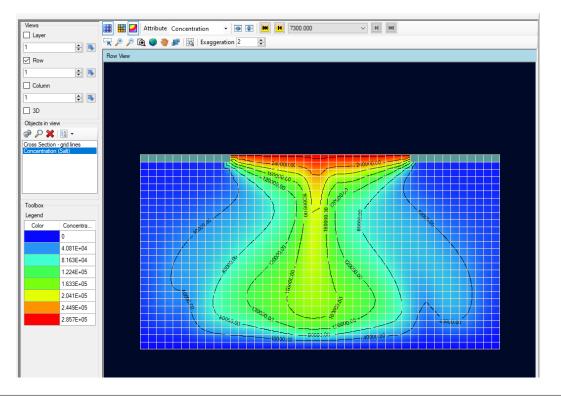
- Click [Translate] directly from the workflow navigator, to return directly to this workflow step
- Go to the [SEAWAT] > [Solvers] section of the menu
- Type: 0.01 in the Residual criterion (RCLOSE) field
- Go to the [SEAWAT Transport] > [Solution Method] section of the menu
- Select Total Variation Diminishing (TVD) in the Advection Method field
- Type: 20 in the Max. number of outer iterations field
- Type: 100 in the Max. number of inner iterations field
- Type: 1E-09 in the Relative Convergence Criterion field

Now re-translate and re-run the model

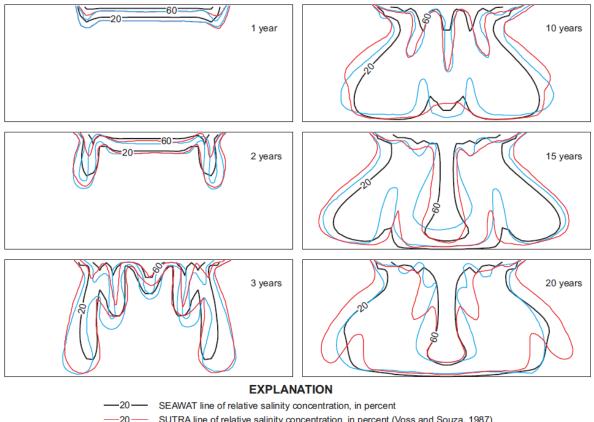
- Click [Translate] directly from the workflow navigator, to return directly to this workflow step
- Click [No] to dismiss the warning(s) about No package data
- Click [Yes] to dismiss the warning about initial heads
- Click [] (Next Step) to proceed to the Run step
- Click [Run] to run the SEAWAT model

When the model is finished running you should see the following results for salt concentrations at day 365 and 7300, respectively. You can also double-check salt concentrations throughout layer 2 to ensure that no negative concentrations are present:





Compare the contours at day 365 and 7300 to the following published results (Guo and Langevin, 2002):



SUTRA line of relative salinity concentration, in percent (Voss and Souza, 1987)

-20-Elder line of relative salinity concentration, in percent (Voss and Souza, 1987)

Comparison between SEAWAT, SUTRA, and Elder's solution for the Elder problem over time.

Figure reference: Guo and Langevin (2002), page 74.

I Note: concentrations in the published results are displayed as a percentage of the constant concentration at the top of the model. In the default Visual MODFLOW Flex output the concentrations are displayed as absolute values.

Now is a good time to save the project. Click [File]>[Save Project] from the main menu.

*****This concludes the 'SEAWAT - Elder Model' tutorial.*****

3.5 PEST with Pilot Points

This section provides instructions on using Visual MODFLOW Flex to setup, run, and interpret a Parameter Estimation/Predictive Analysis simulation. In addition, this tutorial provides a brief description of the input parameters and settings required by PEST. A detailed description of the algorithms, parameters, input files, and other options for PEST are available in the PEST User Documentation, which are available at the PEST website (www.PESTHomepage.org).

This exercise demonstrates some of the advanced and exciting opportunities for model calibration and uncertainty analysis using PEST in Visual MODFLOW Flex. This exercise is based on the problem described in "Using Pilot Points to Calibrate a MODFLOW/MT3D Model" by John Doherty (2008), and has been adjusted to work with the PEST workflow inside Visual MODFLOW Flex.

Pefore you start
You are encouraged to familiarize yourself with the concepts and applications of PEST prior to using in Visual MODFLOW Flex. The time spent on this will make your experience with parameter estimation much more productive, and will likely help you to overcome any difficulties you may experience the first time you run PEST.
In addition, if you are not familiar with the Visual MODFLOW Flex graphical environment, please take a few minutes to review the <u>Program Overview</u> section.
Note:
You must have a Pro or Premium license in order to use the PEST module in Visual MODFLOW Flex.

Objectives

By the time you have finished this exercise you will have:

- used pilot points as a means of characterizing the spatial distribution of an aquifer hydraulic property;
- used PEST's advanced regularization functionality in conjunction with geostatisticallybased regularization constraints;
- used the Visual MODFLOW Flex GUI to:
 - Build input files for PEST
 - o Run PEST

- o Analyze the results
- o Save adjusted parameters as new model inputs

Required Files

Several files are required for this exercise, which are included with the Visual MODFLOW Flex installation. These files are available in the installation documents folder, typically:

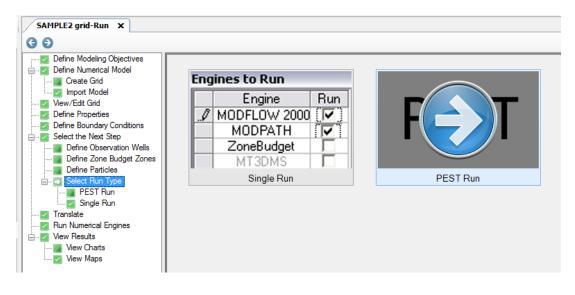
C:\Users\Public\Public Documents\Visual MODFLOW Flex\Tutorials\PEST

If you cannot find these files, please <u>download the PEST Tutorial project from our website</u>, and unzip to a desired folder on your computer.

Introduction

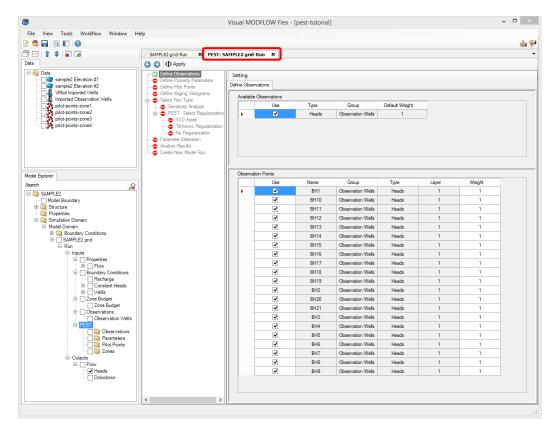
The groundwater model that you will use in this tutorial has already been built. In the first part of the tutorial, you will open the project and start a new PEST workflow:

- Launch Visual MODFLOW Flex
- Click [File]>[Open Project]
- Navigate to your Public 'My Documents' folder, and locate '\Documents\Visual MODFLOW Flex\Tutorials\PEST', and open the 'pest-tutorial.amd' file
- [Open]
- In the Numerical Workflow window, locate the workflow tree (this is shown on the left in the window below)
- If you're not already on this step, click on the 'Select Run Type' in the numerical workflow tree.
- Click on the [PEST Run] button



• A new PEST Workflow window will load as shown below

Please Note: if this does not appear right away, select this tab from the list of workflows across the top of the window, highlighted in image below)



Define Observations

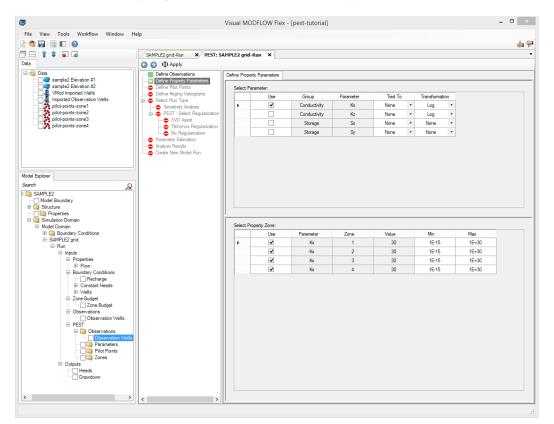
The first step in the PEST workflow is to define the observations you want to include for calculating the objective function, and assign weights to various observations. In this example, there are 21 observation wells where heads were measured at several intervals. These observations were assigned in the main modeling workflow (i.e. the "Sample2grid-Run" workflow) and are automatically added in the PEST workflow. All head observations are selected by default, and will be used with a default weight = 1.

- No changes will be needed at this step for this exercise
- Click [] (Next Step) to proceed to the 'Define Property Parameters' step.

Define Property Parameters

At the Define Property Parameters step in the workflow, you will define which parameters will be included in the objective function, that is which parameters will be adjusted by the PEST

algorithm to reduce differences between observed head values and corresponding simulated head values.



The 'Define Property Parameters' window will appear:

The table at the top of this step allows you to select which property types you want to include as parameters in the objective function. For each parameter, you can specify whether to "Tie" it to another parameter so that it will be varied during the PEST run in relation to the selected anchor parameter. You can also specify a Transformation option (by default, all Conductivity parameters are set to Log transformation) for the parameter sensitivity derivatives.

The table at the bottom of this step allows you to select which specific property zones you want to include in the objective function. For this exercise, all Kx property zones will be included (these are selected by default). You can also specify bounds on the values for each parameter zone:

- Enter 1 for the Minimum for each zone in the lower table
- Enter 300 for the Maximum for each zone in the lower table

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rization			Storage	Sy	None	-	None	-	
Run									
	Select Pro	perty Zone:							
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	Select Pro	Use	Parameter Kx	Zone 1	Value 30		Min 1		Max 300
	Select Pro	Use							
	Select Pro	Use	Кх	1	30		1		300

• Click [] (Next Step) to proceed to the 'Define Pilot Points' step.

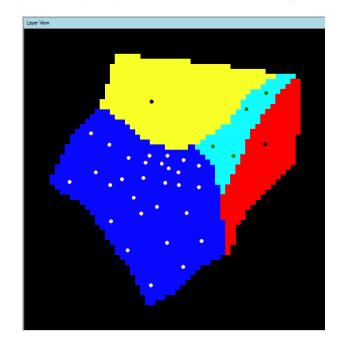
Define Pilot Points

At this step, you will define Pilot Points, which are sets of grid-independent point locations that PEST uses to update model parameters by interpolation (Kriging, discussed in the next section) across specified the specified parameter zones. One set of pilot points is required for each distinct parameter zone: a single pilot point in a parameter zone will result in a homogeneous parameter field for that zone and multiple pilot points in a parameter zone will result in a heterogeneous, continuously distributed parameter field for that zone. The pilot point approach implemented in PEST allows you to methodically determine sets of parameters for your groundwater model that minimize the PEST objective function (e.g. reduce the global differences between observed and simulated values).

• The 'Define Pilot Points' window will appear:

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Pilot points are XY points with an initial value for each parameter. Pilot points can be <u>imported</u> from .TXT file, XLS, .SHP file, or <u>assigned manually</u> by digitizing in the 2D environment. An example of the pilot points on top of conductivity zones is shown below:



The general steps to assign pilot points in the PEST workflow are as follows:

- Select 'pilot-points-zone1' data object from the Data Explorer (tree)
- Click [] (Insert button) at the top of the 'Define Pilot Points' window to add these points.
- Select which parameter zones the points represent under the Parameter Zones grid in the upper right section of the window.
- For this set of pilot points, **Kx-Zone1** is fine (this should be selected by default)
- Your display should now appear as shown below:

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Repeat these steps to define the pilot points for Kx Zone2, Kx Zone3, and Kx Zone 4:

- Select 'pilot-points-zone2' data object from the Data Explorer (tree)
- Click [] (Insert button) at the top of the 'Define Pilot Points' window to add these points.
- Select Kx-Zone2 for these pilot points (if it is not already selected)
- Select 'pilot-points-zone3' data object from the Data Explorer (tree)

- Click [] (Insert button) at the top of the 'Define Pilot Points' window to add these points.
- Select KxZone3 for these pilot points
- Select 'pilot-points-zone4' data object from the Data Explorer (tree)
- Click [] (Insert button) at the top of the 'Define Pilot Points' window to add these points.
- Select Kx-Zone4 for these pilot points
- When you are finished, your display should appear similar to the figure below.

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I II										

In the table at the bottom of the window, you can adjust some parameters for specific pilot points. Above this table, there is a combo box that allows you to select which set of pilot points is shown in the table based on the selected parameter zone.

The main use of this table is to specify initial values for the pilot points in each parameter zone and which of these pilot points will be used and/or set as "Fixed" during subsequent PEST runs. Fixed pilot points are those locations where you are confident in the measured parameter value (e.g. based on pumping/slug test locations) and you want these values to remain unchanged during the PEST run.

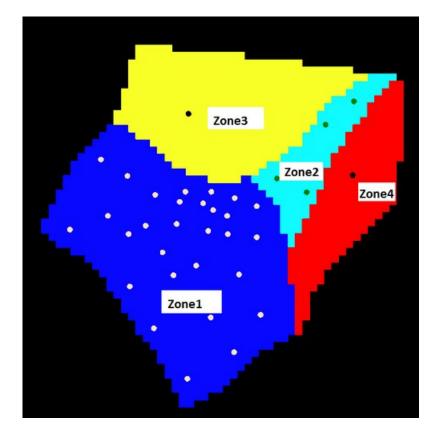
In this example, leave the defaults as is.

• Click [] (Next Step) to proceed to the Define Kriging Variograms.

Define Kriging Parameters

The use of pilot points in characterizing the spatial distribution of a hydraulic property must be accompanied by a mechanism whereby hydraulic property values assigned to pilot points are spatially interpolated to the cells of the finite difference grid. In PEST, this spatial interpolation is accomplished using the Kriging algorithm. Kriging is a method of spatial interpolation from the field of geostatistics. The cornerstone of geostatistics is the variogram. A variogram describes the extent to which hydraulic property values (or any other type of data) pertaining to any two points are likely to be different from each other as a function of the distance between those points.

One of the benefits of using Kriging as a basis for spatial interpolation is that the factors by which hydraulic properties at pilot points are multiplied before summation to obtain the hydraulic property value at a particular grid cell are independent of the actual hydraulic property values at the pilot points. Hence a set of "Kriging factors" pertaining to each of the cells of the finite difference grid can be calculated in advance of the actual interpolation process. Since the interpolation process is undertaken again and again as the model is run repeatedly by PEST, the fact that it is not necessary to repeat calculation of the Kriging factors on each occasion that the model is run can result in large savings in the time required to complete the overall parameter estimation process.



In this example, there are 4 hydraulic property zones as shown below:

- Zone 1: River Alluvium
- Zone 2: Creek Alluvium

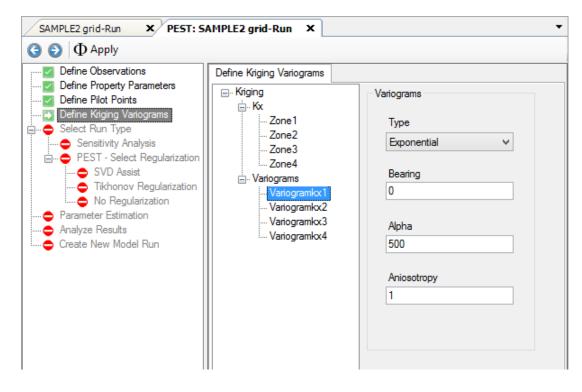
- Zone 3: Western Basalt
- Zone 4: Eastern Basalt

Each zone is represented by a geostatistical structure. Each of these structures cites one variogram (though it could cite up to five, one for each groundwater flow property: Kx, Ky, Kz, Ss, Sy). In this tutorial:

- "Structure1" will be used to characterize Zone 1 of our model domain (i.e. the river alluvium),
- "Structure2" will be used to characterize Zone 2 (i.e. the creek alluvium),
- "Structure3" will be used to characterize Zone 3, and
- "Structure4" will be used to characterize Zone 4 (i.e. the eastern basalt).

Note that the variogram assigned to these zones 3 and 4 is not important: because there is only one pilot point assigned to each of them, all cells within these zones will be assigned the one interpolated value (same as the respective pilot point) irrespective of the variogram. Assigning a single pilot point to a given zone is effectively the same as the approach that was standard in older versions of PEST where hydrogeologic properties were homogenous within a zone.

In Visual MODFLOW Flex, a default variogram is generated for each parameter zone, based on a type 2 (Exponential) distribution.



However, the structures should be verified/modified.

• Click 'Zone1' under 'Kx' in the tree. The display will appear as below:

G 🕤 Φ Apply	
 Define Observations Define Property Parameters Define Pilot Points Define Kriging Variograms Select Run Type Select Run Type Select Regularization SVD Assist Tikhonov Regularization No Regularization No Regularization Analyze Results Create New Model Run 	Structure Nugget 0 Transform log V Number of Variograms 1 Weight 0.15 Kriging Min. Number of Points 1 Max. Number of Points 50 Search Radius 2000

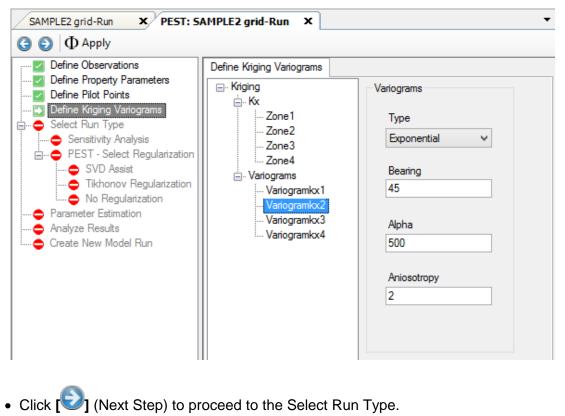
- In the editor on the right side of the display, for 'Transform', set this to log.
- Repeat these steps, setting log 'Transform' for Kx in Zones 2, 3, and 4.

Any variogram cited in each of these structures will pertain to the spatial distribution of the logarithm of the pertinent hydraulic property. This is in accordance with the fact that most studies cited in the groundwater literature which treat transmissivity and/or hydraulic conductivity as a regionalized variable indicate that its distribution is better described by a log variogram than by a variogram based on native property values.

For this example, the default parameters for the variograms (all will use Exponential) is sufficient. However, for Zone2, we will define a value of 2.0 for the Anisotropy, with the direction of anisotropy coinciding with the direction of the creek. Alignment in the direction of the creek is based on the premise that channel structures within this old creek valley will make it more likely for hydraulic property similarity to prevail in this direction than in a direction at right angles to it.

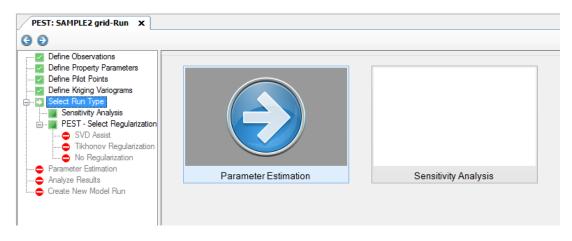
The variogram parameters can be adjusted by selecting a Variogram from the tree as shown below:

- Click 'Variogramkx2' under the Variograms node in the tree.
- Enter 2 for the 'Anisotropy'.
- Enter 45 for the 'Bearing'. This value allows you to make the variogram anisotropic in a certain direction; 'Bearing' is an angle of rotation specified in degrees counterclockwise from the positive X-Axis (East).
- The display should appear as below:



Select Run Type

At this step, choose the type of PEST Run. If you want to run PEST, then some additional options will be needed, such as define regularization and adjust the PEST control file. If you want to run Sensitivity Analysis, this can also be launched.



- Click the [Parameter Estimation] button from the main window, as shown above.
- The next step will be to choose the Regularization options.

Select Regularization

At this step, you can choose the type of Regularization to run. Regularization is a process whereby additional information is introduced into the objective function of the model in the form of 'prior information equations'. These prior information equations can take many forms:

- **Tikhonov Regularization** can induce PEST to prefer a more homogeneous solution (i.e. pilot points that in the same parameter zone should have similar values) or to prefer parameter values which are as close to their initial values as possible. The Tikhonov regularization method adds more information to the overall problem, but the additional information helps to guide PEST toward acceptable parameter estimates as informed by your knowledge of the modeled area and helps to avoid 'overfitting' solutions.
- Singular value decomposition (SVD) regularization achieves numerical stability in PEST by subtracting parameters or combinations of parameters from the calibration process. As a result of the subtraction, the calibration process is no longer required to estimate either individual parameters or combinations of correlated parameters that are inestimable on the basis of the calibration dataset. These combinations are automatically determined through singular value decomposition (SVD) of the weighted Jacobian matrix.

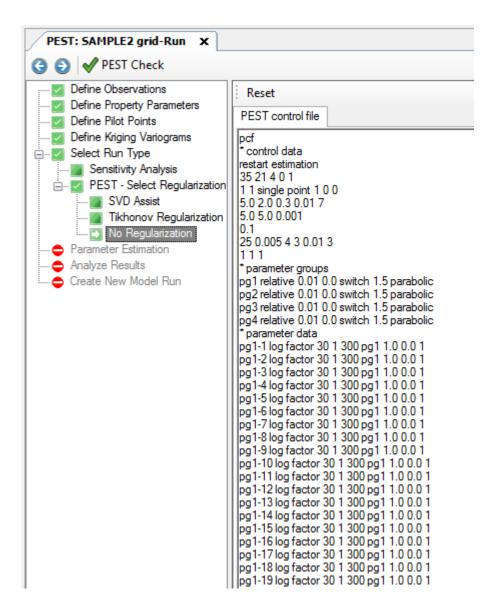
For this exercise we will not perform any regularization.

PEST: SAMPLE2 grid-Run X		
G		
 Define Observations Define Property Parameters Define Pilot Points Define Kriging Variograms Select Run Type Senstivity Analysis PEST - Select Regularization SVD Assist No Regularization Parameter Estimation Analyze Results Create New Model Run 	No Regularization	Tikhonov Regularization
	SVD Assist	

- Click [No Regularization] button from the main window
- The next step will be to adjust the PEST control file.

Edit PEST Run Settings

The last step before running PEST is to review and adjust the PEST Control file.



If you are familiar with the PEST file format/structure, you can adjust the PEST Control file in this window, or copy into a text editor, make changes, and paste the adjusted contents back in this window. A full explanation of the PEST control file is available in the PEST <u>manual</u>. For this exercise, the default values are fine.

Before starting the PEST Run, it is a good idea to check the PEST Input files. PEST provides a utility to do this, called PESTCheck.

- Click the [PEST Check] button on the workflow toolbar
- You should receive a confirmation that no errors were found.
- Click [OK] to proceed.
- Click [[(Next Step) to proceed to the Run PEST window.

Run PEST

At this step in the workflow, you will run PEST:

Run PEST

Click [] (Run F

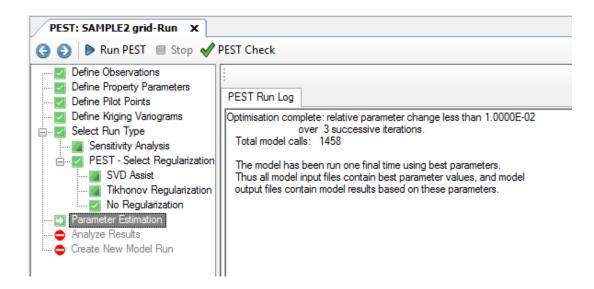
] (Run PEST) to start the PEST Run.

The PEST program (pest.exe) will load in a DOS command window, and show the progress as seen below.

C:\windows\system32\cmd.exe -	×
C:\Users\bmcneill\Work Folders\Training\pest-tutorial.data\MODFLOW\SAMPLE2 gri Run\MODFLOW-2000>"C:\Program Files\Visual MODFLOW Flex\pest.exe" pest_run.pst	id\ ^
PEST Version 12.3.1. Watermark Numerical Computing.	
PEST is running in parameter estimation mode.	
PEST run record: case pest_run <see details.="" file="" for="" full="" pest_run.rec=""></see>	
Model command line: model.bat	
Running model	
Running model 1 time Sum of squared weighted residuals (ie phi) = 1203.7	
OPTIMISATION ITERATION NO. : 1 Model calls so far : 1 Starting phi for this iteration: 1203.7	
Calculating Jacobian matrix: running model 35 times 21 runs completed.	¥

Depending on the speed of your computer, the PEST run should take between 3-5 minutes. Note that the groundwater model used in this tutorial is relatively small and has relatively few parameters - PEST runs involving larger models with longer run times and many parameters may take considerably more time: up to several days or even longer in more extreme cases. As PEST runs, you should see the objective function (phi) decreasing over each optimization iteration; pay attention to these values in the DOS window. In this tutorial, PEST will run a total of 25 optimization iterations and a total of approximately 1400 model runs. PEST should reach a final objective function (phi) value of approximately 5E-03.

When PEST finishes, you should see a confirmation message in the main window, below the **'PEST Run Log'** tab, as shown below.



After the PEST run completes, you can analyze the results.

• Click [] (Next Step) to proceed to the 'Analyze Results' step.

Analyze Results

Visual MODFLOW Flex will present the results of the PEST run, with one tab per output file:

250

PEST: SAMPLE2 grid-Run X		
G 🕤 🧏 Export		
Define Observations	PEST.REC PEST.SEO PEST.SEN PEST.RES	
Define Property Parameters Define Pilot Points Define Kriging Variograms	PEST RUN RECORD: CASE pest_run	
Select Run Type	PEST Version: 12.3.1	
SVD Assist	PEST run mode:-	
No Regularization	Parameter estimation mode	
Parameter Estimation Analyze Results Create New Model Run	Case dimensions:-	
	Number of parameters : 35 Number of adjustable parameters : 35 Number of parameter groups : 4 Number of observations : 21 Number of prior estimates : 00	
	Model command line(s):-	
	model.bat	
	Jacobian command line:-	
	na	
	Model interface files:-	
	Templates: pest.kx.points.tpl for model input files: pest.kx.points.dat	
	(Parameter values written using single precision proto (Decimal point always included.)	ocol.)
	Instruction files: pest.heads.ins for reading model output files: pest.mod2obs.out	
	PEST-to-model message file:-	
	na	

- Record file (.REC): contains parameter values, objective function, sensitivities, etc..
- Sensitivities for Observations (.SEO): contains the observed and simulated values with the sensitivities
- Sensitivities for Parameters (.SEN): provides the information on parameter sensitivities
- Residuals (.RES): contains the adjusted calculated vs. observed values and residuals

The results from these files can be exported into Excel for charting.

Click [^{Secont}] to export the PEST results to an Excel spreadsheet.

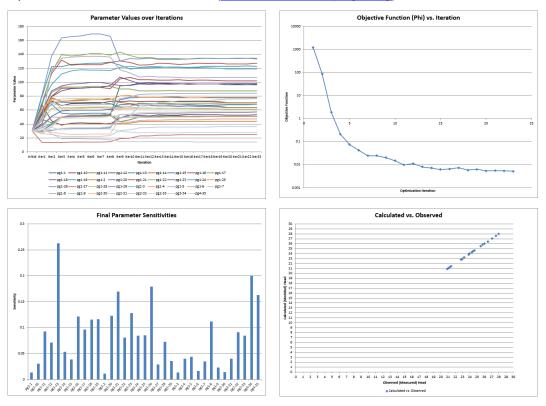
A window will appear which allows you to select the location of the exported Excel spreadsheet, and to select from available templates. Two templates are available; one which will export the available PEST data to a series of worksheets/tables, and a 2nd template which will also generate a number of charts for each type of PEST data.

- Select the 'pest-results-chart-and-table.xlsx' template
- Click the checkbox besides 'Open file when finished'

- Select an output location
- Click Export; the Export Pest Results window should look like the image below before exporting:

>	Export	PEST Results	×
Template:			
Edit	Rename	Clone	× 18
Output File: C:\Users\bmc	neill\Desktop\pest-resu	ts xlsx	
	/hen finished		

An Excel spreadsheet will open which summarizes the results of the PEST run. Several data tables and charts are included; spend a few minutes reviewing them. The screenshots below display a small selection of the available PEST data. For more information about the PEST results please visit the PEST website (www.PESTHomepage.org).



If the results look reasonable, you can save the adjusted Kx parameter zonation as inputs for a new model; this is explained in the next section.

• Click [] (Next Step) to proceed.

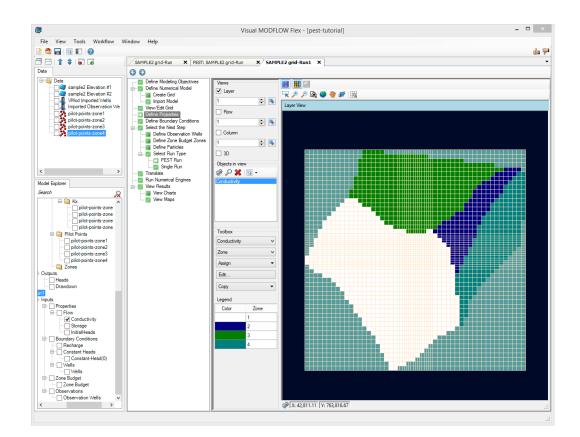
Save PEST Parameters as New Inputs

After reviewing the PEST output, if the adjusted parameter values seem reasonable, you can save these parameters as inputs for a new model run.

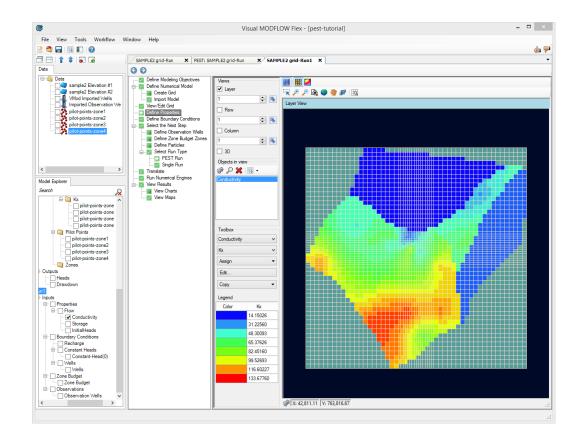
PEST: SAMPLE2 grid-Run X		
G D		
 Define Observations Define Property Parameters Define Pilot Points Define Kriging Variograms Select Run Type Sensitivity Analysis SYD Assist SVD Assist No Regularization Parameter Estimation Analyze Results Create New Model Run 	Create New Model Run Create N	ew Model Run With PEST Results

• Click on the [Create New Model Run with PEST Results] button.

Visual MODFLOW Flex will save the adjusted model parameters in a new model run within the same project. This new model run will appear in the Model Explorer below the most recent model run. A new workflow window will also appear with this model run.



- Click on 'Define Properties' from the workflow tree (if not already selected)
- From the Toolbox, select **'Kx'** as shown below; you should then see a color flood of the Kx values.



You can mouse over the 2D display to see the range of Kx values. Click on the I button on the toolbar to show color shading with contour lines.

You must Translate and Run this new model run in order to see the updated MODFLOW results using the adjusted Kx parameters from PEST.

*****This concludes the 'Model Calibration Using PEST with Pilot Points' tutorial.*****

3.6 MODFLOW-USG Tutorial

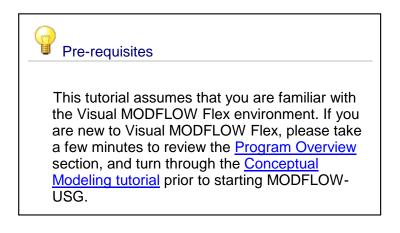
The following example is a walk through of creating a MODFLOW-USG groundwater flow model. The exercise is based on a conceptual model project that is already defined in one of the Tutorial projects.

Objectives

• Open and review a VMOD Flex project that contains a conceptual model

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- Define UnStructured Voronoi and Quadtree Grids (V-Grids and Q-grids), with refinement around wells, boundaries and other features of interest
- Convert a conceptual model to a numerical model
- View the corresponding flow properties for the MODFLOW-USG model
- View the boundary condition cells for MODFLOW-USG model
- Translate and Run MODFLOW-USG
- View and Analyze the Results
- Understand how Visual MODFLOW flex accommodates inputs and outputs for a MODFLOW-USG model



Required Files

Several files are required for this exercise, which are included with the Visual MODFLOW Flex installation. These files are available in the installation documents folder, typically:

C:\Users\Public Documents\Documents\Visual MODFLOW Flex\Tutorials\MODFLOW-USG\Transient\

If you cannot find these files, please <u>download a copy from our website</u>, and unzip to a desired folder on your computer.

Review the Conceptual Model

The surficial geology at the site consists of an upper sand and gravel aquifer, a lower sand and gravel aquifer, and a clay and silt aquitard separating the upper and lower aquifers. These are defined as three property zones in the conceptual model, with hydraulic conductivity for the aquifer as 2E-04 m/s and the aquitard having a horizontal conductivity of 1E-10 m/s and vertical conductivity (Kz) = 1E-11 m/s.

Initial heads are defined using the Ground surface, and this value is applied to all layers.

The boundary conditions consist of a constant head in upper aquifer, in the north part of the model, a river along the southern edge, and two pumping wells screened over the bottommost property zone, each pumping 400 - 700 m³/day, with a time-varying pumping schedule. Constant head values are also defined in the lower aquifer. Each boundary condition consists of a few simple stress periods to illustrate a transient MODFLOW-USG model run.

When discussing the site, in plan view, the top of the site will be designated as north, the bottom of the site as south, and the left side and right side as west and east, respectively. Groundwater flow is from north to south (top to bottom).

Opening the Project

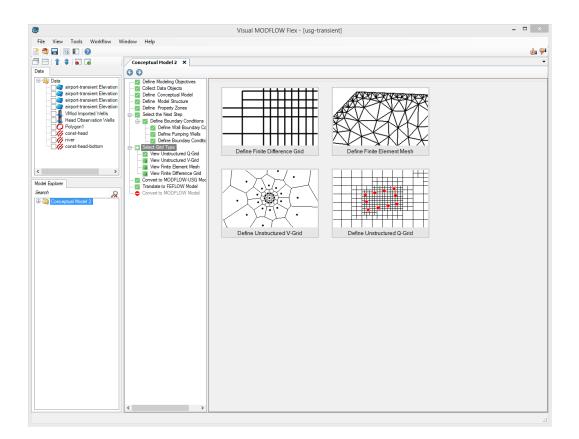
The conceptual model discussed above that you will use in this tutorial has already been built in a Visual MODFLOW Flex project for you. In the first part of the tutorial, you will open the project:

- Launch Visual MODFLOW Flex
- Click [File]>[Open Project...]
- Navigate to your 'Public Documents' folder then locate 'VMODFlex\Tutorials\MODFLOW-USG\Transient\'
- Open this folder, select the 'usg-transient.amd' file.
- Select [Open]
- The project will load.

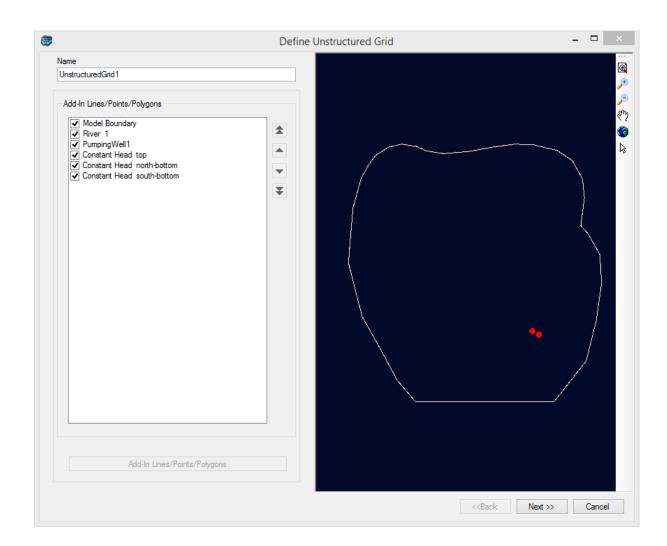
Define an UnStructured V-Grid

At this step in the tutorial, you will define an unstructured Voronoi grid (V-grid) for the model. Voronoi grids are tessellations of the model domain (in plan view) using irregularly-shaped convex polygons based on a set of input add-in vertices associated with important features in the conceptual model. To start the process:

- Select the **'Conceptual Model 2'** tab (from the list of active workflows/windows, at the top of the display)
- Navigate to the 'Select Grid Type' step in the workflow (if its not already selected), as shown below.



• Click on the 'Define UnStructured V-Grid' button, and the following window will appear:



The first step in defining the unstructured Voronoi grid (V-Grid) is to specify the input shape add-ins. Shape add-ins are polylines, polygons, and points within the model boundary. The V-Grid generator in Visual MODFLOW Flex will use these as control points (grid generator nodes) when creating the unstructured grid. By default, the Add-ins List contains the model boundary (polygon) and any linear or point boundary condition currently defined for the conceptual model. Additional add-ins may be added to the list by selecting data objects from the Data Explorer, and then clicking on [Add-In Lines/Points/Polygons] button (For example, you may want to add-in the points that represent your head observations (targets), so that these will be located in the (horizontal) center of an unstructured grid cell. Likewise, you can conform the grid around geological features such as faults/fractures). An Add-in may be included or excluded in the grid creation, by checking or unchecking the corresponding check box, respectively. When an add-in is "checked" it will also be displayed in the adjacent 2D Viewer preview window.

• Click the [Next>>] button to proceed.

In the second dialog, you can define various discretization settings for the horizontal grid and adjust refinement levels and smoothing around the line and point add-ins.

(2)	Define Unstructured Grid -		
Name UnstructuredGrid1 Define Unstructured Grid Delaunay Triangulation Method (L-switch) Force all triangles to be Delaunay Meshing Algorithm (i-switch) Divide and conquer Image: Total number of elements (Approx) 1000 Quality mesh (q-switch), minimum angle (0-30 degrees) 30 Refinement Image: Refinement along all superelement border edges Target element edge length 19.2 Image: Refinement along line add-ins Target element edge length 19.2 Image: Refinement around point/well add-ins Number of triangles around points 10 Space from points to new nodes 4.3 Gradation: steep Image: Layer Refinement Settings	Define Unstructured Grid	۵ ۱ ۲))))
Triangle - Copyright (c) by J.R. Shewchuk, v.1.6 (2005)			
	Generate < <back finish<="" td=""><td>Cancel</td><td>]</td></back>	Cancel]

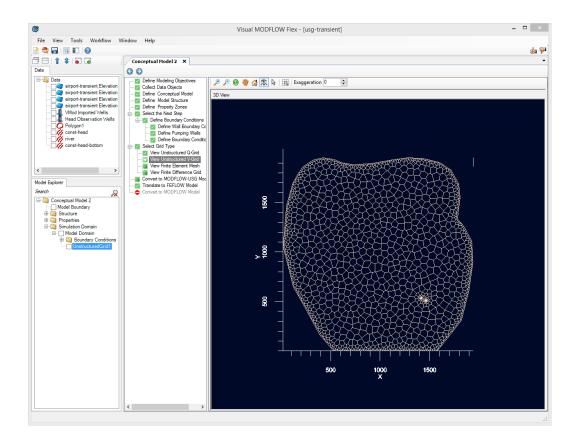
For now, you will just use the default settings. However, you may find it a useful exercise to create a copy of the project and experiment with these settings.

• Click the **[Generate]** button (located in the bottom middle section of the window). A preview of the V-grid will appear in the adjacent 3D viewer. If you are not satisfied with the grid, you can modify the settings and regenerate the grid by selecting the Generate button again.

(***)	Define Unstructured Grid – 🗖 🗙
Name UnstructuredGrid1 Define Unstructured Grid Delaunay Triangulation Method (L-switch) Force all triangles to be Delaunay Meshing Algorithm (i-switch) Divide and conquer Total number of elements (Approx) 1000	Define Unstructured Grid - X
Quality mesh (q-switch), minimum angle (0-30 degrees)	
Refinement ✓ Refinement along all superelement border edges Target element edge length 19.2 ✓ Refinement along line add-ins Target element edge length 19.2 ✓ Refinement around point/well add-ins Number of triangles around points 10 Space from points to new nodes 4.8 Gradation: steep	
Layer Refinement Settings Mesh exterior boundary edges: 343	
Mesh interior boundary edges: 0 Mesh subsegments (constrained edges): 343 Triangle - Copyright (c) by J.R. Shewchuk, v.1.6 (2005)	Generate < <back cancel<="" finish="" td=""></back>

• Click [Finish] to generate the numerical grid and close the window.

The Unstructured V-Grid will be added as a new data object to the Conceptual Model tree, under the Simulation Domain folder, and should appear as shown below with the name **UnstructuredGrid1**.

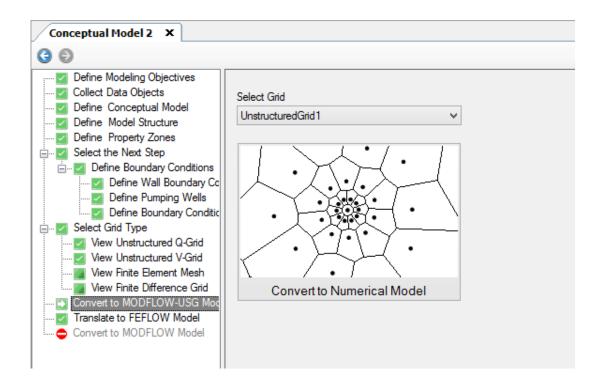


• Click [] (Next Step) to proceed.

Generate the Numerical Model

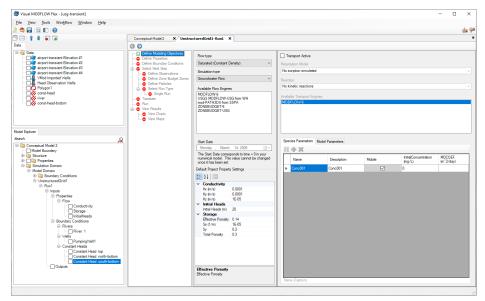
You should arrive at the 'Convert to MODFLOW-USG Model' workflow step. You are now ready to create a numerical model from the unstructured grid you created, using the property zones and boundary conditions defined in the conceptual model.

- Click the 'Convert to MODFLOW-USG Model' step in the list of workflow steps (if you're not already there)
- Click the [Convert to Numerical Model] button

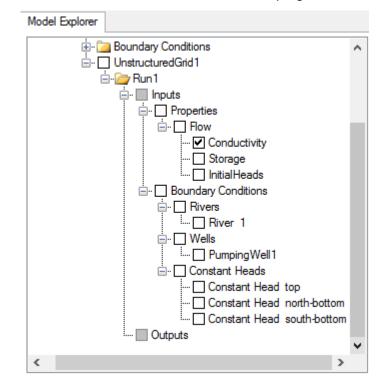


The conversion process will begin; this may take a few moments. Note that for larger grid sizes and more complex boundary conditions, this conversion process may take several minutes.

After the conversion is complete, a new workflow tab will appear, titled "UnStructuredGrid1-Run1". This workflow will provide you the tools and displays for navigating the MODFLOW-USG Numerical Model (keeping in mind that you were previously navigating and working with a Conceptual Model). More details on the specifics of each step can be found in the section <u>MODFLOW-USG Numerical Modeling Workflow</u>.



In addition, you will now see new items in the Model Explorer, under the UnstructuredGrid1 node (in the lower left corner of your window), with a Run folder containing Inputs (Properties and Boundary conditions) and Outputs (which will be added after a successful run). For the boundary conditions, you will see nodes for groups of boundary condition cells that were generated: Constant Head boundaries, River, and the Pumping Wells.

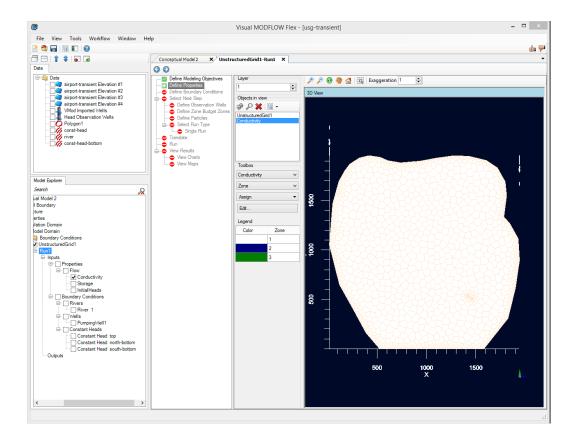


Define Properties

The first step that appears in the workflow is Define Modeling Objectives step. This step allows you to define type of model which will be run and to define many default property values. These values should be identical to the values initially defined in the 'Define Modeling Objectives' step during the conceptual modeling workflow. For now we will retain all the default values.

• Click [] (Next Step) to proceed.

The Define Properties workflow step will appear, which lets you edit Conductivity, Storage, and Initial Heads values in your numerical model.



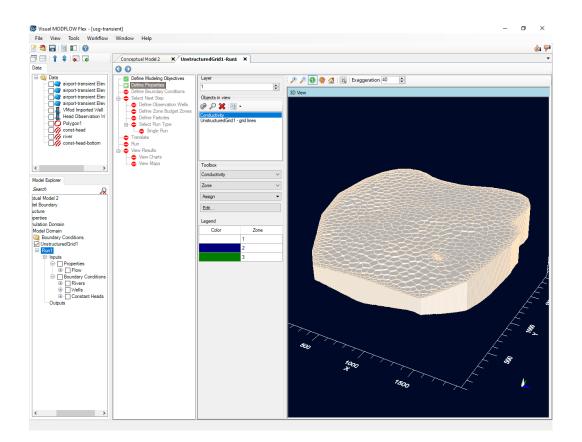
By default, Conductivity will be displayed in the 3D viewer and unstructured grid cells in the uppermost layer (Layer 1) will be rendered and colored by property zone.

In order to gain a better perspective, you need to apply a Vertical Exaggeration and rotate the 3D Viewer.

- Locate the 'Exaggeration' field in the toolbar above the 3D Viewer
- Type: 40, then press Enter on your keyboard.

Now you will rotate the 3D view to see the property zones from a side-view perspective. Above the 3D Viewer, you will see a set of standard navigation tools for zoom in/out, pan, and rotate which you can use to further manipulate the view.

- Select the rotate [199] button in the toolbar
- · Left-click with the mouse near the bottom middle section of the 3D display
- Hold down the left-mouse button, and drag your mouse upwards towards the top of the VMOD Flex window, then release the mouse button. By clicking and dragging the mouse in the viewer window you can position the image however you like. You can also use <u>keyboard shortcuts</u> to navigate with more precision.



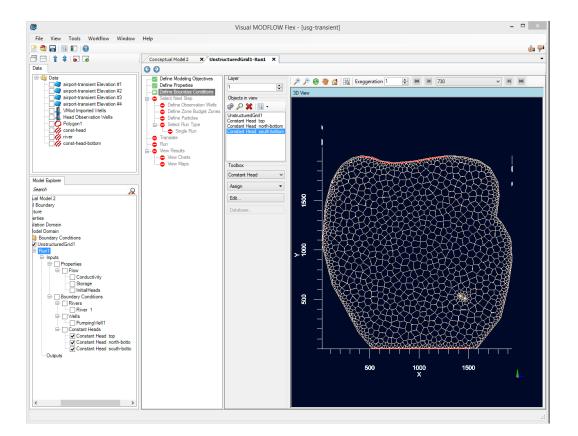
In order to change how the parameter values are displayed, you need to load the settings. (These steps are optional in the Tutorial exercise): Right-click on **'Conductivity'** in the Model Explorer, and select **[Settings]**. This will allow you to render by the parameter value (eg. Kx) instead of by ZoneID, and also show cross-sectional slices and color maps. Take a moment to experiment with these <u>Settings</u>, and when you are finished, click the **[OK]** button to close the Settings.

In order to see another parameter group, you need to de-select (remove the checkbox beside) Conductivity in the Model Explorer, then select (add a check-box beside) the new parameter group, eg. Initial Heads. Take a moment to experiment with these options.

• Click [] (Next Step) to proceed.

Define Boundary Conditions

At this step in the workflow, you can see and edit the numerical (cell) representations of the Boundary Conditions that were generated from the conceptual model objects. The constant heads on the north and south boundaries are shown as red cells, the river is shown as blue cells, and the pumping wells are beige. You display should now appear similar to the image below:



Take a moment to zoom into the river and constant head cells to see the boundary condition cell geometry. You may need to switch layers to see the boundaries.

Each boundary condition will be colored differently. All wells and line-based boundary conditions will be shown by default.

The display settings for a group of boundary condition cells can be adjusted through the settings. We will turn on the Cell ID for the well cells.

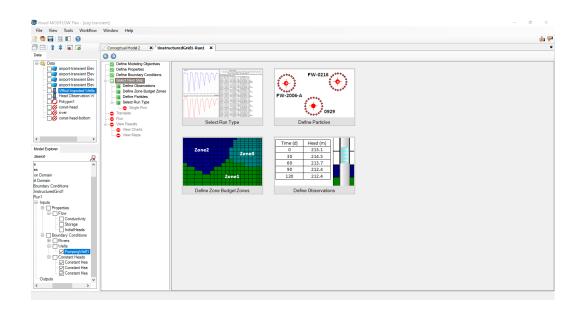
- Locate 'PumpingWell1' in the Model Explorer, under 'Run1/Input/Boundary Conditions/Wells'
- Ensure 'PumpingWell1' is being displayed by activating the checkbox (b)
- Right click on this item and select [Settings...]
- Select [Style]>[Cells] in the Settings tree on the left side of the dialog
- · Check the box beside 'Show Cell ID labels'
- Click [OK]

You should now see the Cell ID drawn beside the two well cells in the 3D viewer. If these are hard to read, try changing the grid color by editing the 'UnstructuredGrid1' settings. You can also change the background color by right-clicking in the 3D viewer and selecting 'Background Color'. You will need to zoom into the two pumping wells in order to see the Cell ID label. The Cell ID can assist when editing the numerical values, or when cross-checking the values in the .WEL package. For more details on editing the numerical values for boundary conditions, see <u>View and Edit Boundary Conditions</u>

• Click [] (Next Step) to proceed.

Optional Model Elements

You should now see the 'Select Next Step' workflow step. At this stage, in addition to proceeding to translating and running the model, you can define several optional model elements such as particles (for mod-PATH3DU simulations), Zone Budget Zones (for ZoneBudget-USG simulations), and observation wells (for calibration charts). In this tutorial, we will add each of these elements in the sections below.

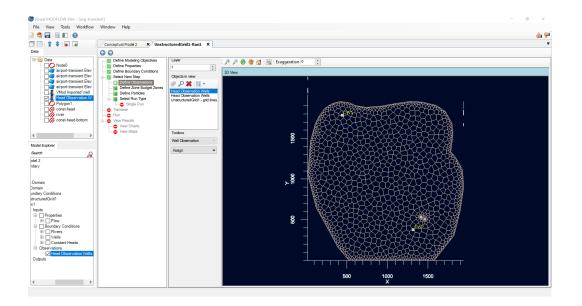


Define Head Observations

We will map the head observation wells (raw data) to the numerical model, so that this data can be used for model calibration. From the 'Select Next Step' workflow window, select the 'Define Observation' option:

- Click the 'Define Observation' button
- Select the **'Head Observation Wells'** data object from the Data Tree in the top-left panel of the window.
- Next, ensure that 'Well Observation' is selected from the first dropdown menu under the 'Toolbox' section.
- Click [Assign]>[Using Data Object] from the toolbox. Click on the [
- Click [OK].

The observation wells will be added to the display and the Model Explorer. These will appear as two green points, one is located in the top left corner, the other in the bottom right corner.



Please Note: some display settings have been changed from the default values in the image below; vertical exaggeration set to 0, observation well points increased size).

Define Zone Budget Zones

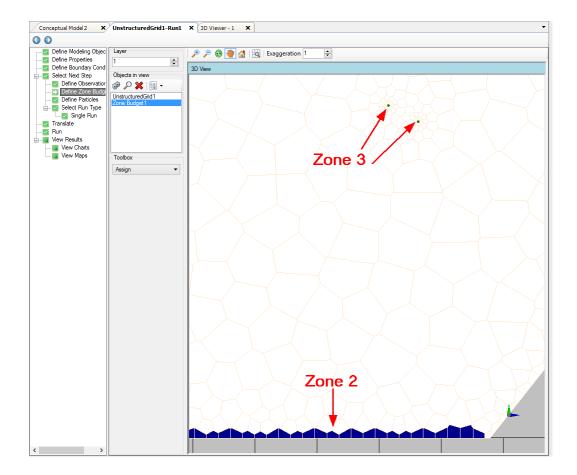
It is also possible to define Zone Budget zones for unstructured grid models. To do this, you will return to the 'Select Next Step' workflow step, and select 'Define Zone Budget Zones' option, or click this step directly in the workflow menu. You will then define a zone budget zone for our pumping wells, so that we can estimate the volume of water pumped extracted the course of the simulation. We will also assign a zone budget zone to the cells which contain the river boundary condition (i.e. southern boundary).

- Click the 'Select Next Step' workflow step in the workflow navigator
- Click the 'Define Zone Budget Zones' button
- Under the toolbox, click 'Assign' > 'Using data object...'
- From the 'Data Tree' select the 'river' data object
- Click on the [
- Click OK
- The 'Create new zone budget zone' window will appear
- Click 'New' to create a new zone budget zone (i.e. Zone 2, blue)
- Ensure that **all** layers (including **'Layer 2'** and **'Layer 3')** are selected in the 'Assign to layer' frame

Cre	ate new zone budget zone 🛛 🗙
	Assign to single zone Select zone:
	Zone 2 V New
\bigcirc	Create new zones from attribute
	No attributes \sim
	Use integer field values
As	sign to layer Assign to all layers
NN	Layer 1 Layer 2
	Layer 3
	OK Cancel Help

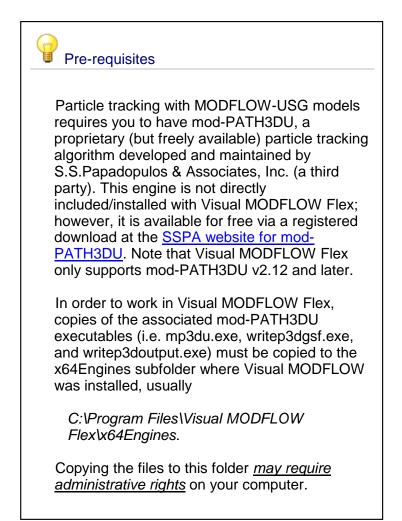
- Click OK
- · Now assign the zone budget zone for our pumping wells
- Zoom to the location of the pumping wells (lower-right corner)
- Under the toolbox, click 'Assign' > 'Single'
- Click both cells containing pumping wells (i.e. the two central cells that have been refined around)
- Click 'Finish' under the toolbox
- Click 'New' to create a new zone budget zone (i.e. Zone 3, green)
- Ensure that **all** layers (including **'Layer 2'** and **'Layer 3')** are selected in the 'Assign to layer' frame
- Click OK

In the Model Explorer, you can activate the 'Zone Budget1' object to display the distribution of zone budget zones. If you turn this object on and zoom to the lower-right corner of the model you should be able to view all three zone budget zones at once (see image below):



Define Particles

At this step you can define particles to be used in particle tracking simulations using mod-PATH3DU.



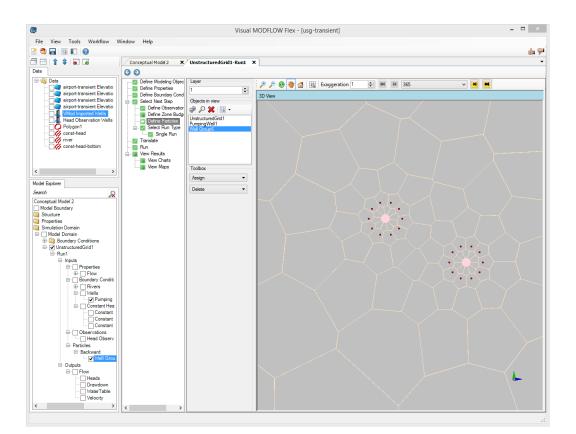
Let's define some backward tracking particles around our pumping well objects. These will help us to delineate a capture zone for these wells.

- Click 'Define Particles' in the 'Select Next Step' workflow window
- Under the toolbox, click 'Assign' > 'Using well object...'
- The 'Create New Particles' window will appear
- In the Data Tree select the 'VMOD Imported Wells' data object
- Click on the [] button where it says 'Select object'
- In the 'Particles along screen' field, specify '3' as the '# of Circles'
- When you're finished, the 'Create New Particles' window should look like the image below:

💭 Create New Particles		_		\times
Particle group name Well Group Select object Image: Select object Image: VMod Imported Wells Particles on circle Radius: (m) 10 Image: # Particles 10	Particle propagation Forward Backward Release time Beginning of simulation End of simulation Custom 0			
Particles along screen # Circles 3	ОК]	Cancel	

• Click 'OK' to define the particles

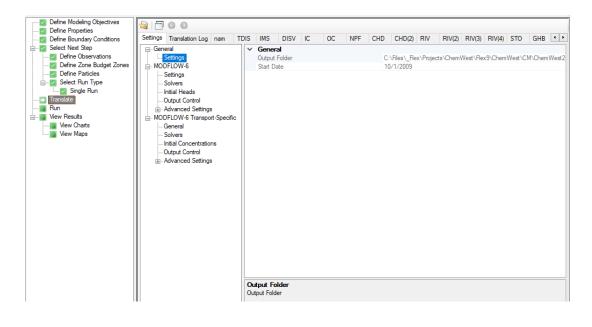
You should see a circle of particles appear around the pumping wells in the lower-right corner of the model, as shown below (note: background color changed, and image is zoomed to location of the particles):



- Click [] (Next Step) to proceed to the 'Select Run Type' workflow step
- Click [] (Next Step) to proceed to the 'Single Run' workflow step
- Select USGS MODFLOW-USG from WH as the Flow Engine, if it isn't already
- Activate Zone Budget and particle tracking:
- ZONEBUDGET-USG
- 🗹 Particle Tracking
- Click [[(Next Step) to proceed to the 'Translate' workflow step

Translate (Create MODFLOW-USG Input files)

At the Translate step, you create the packages for MODFLOW-USG, and you can preview and make adjustments to the input files where needed.



- Under 'MODFLOW-USG' > 'Settings' > 'Run Type', select 'Transient'
- Click [Translate] to create the MODFLOW-USG packages.

The translation will begin, it should complete in approximately 5-10 seconds. At this stage, if any errors or warnings are encountered with any of the packages, you will be notified. Take a moment to preview the MODFLOW-USG input files; each package will appear as a separate tab across the top of the window.



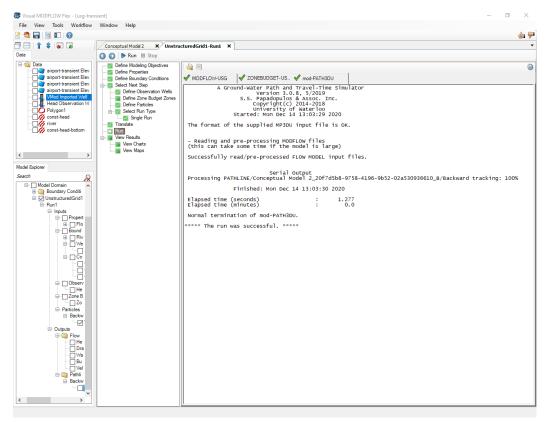
- When you are finished, you can proceed to the run step.
- Click [] (Next Step) to proceed to the 'Run' workflow step

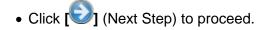
Run MODFLOW-USG

At this step in the tutorial, you will run the model:

• Click the [PRINT] button to run MODFLOW-USG.

The MODFLOW-USG Engine will start running and show progress of the model run in the main viewer window. After the model run completes, you can view the summary of the mass balance for the last time step in each stress period, by clicking on the the MODFLOW-USG tab.





View Maps Step: Visualizing Model Outputs

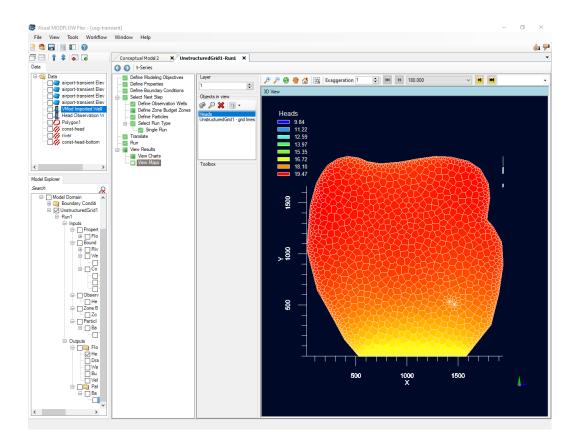
At this step in the tutorial, you will visualize the model results

Viewing Output Heads

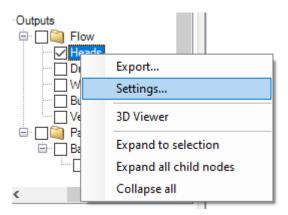
The first type of model result you will review is the output heads

• Click the [View Maps] button when presented with the desired results options.

You will then see cell rendering of calculated heads in the 3D Viewer:



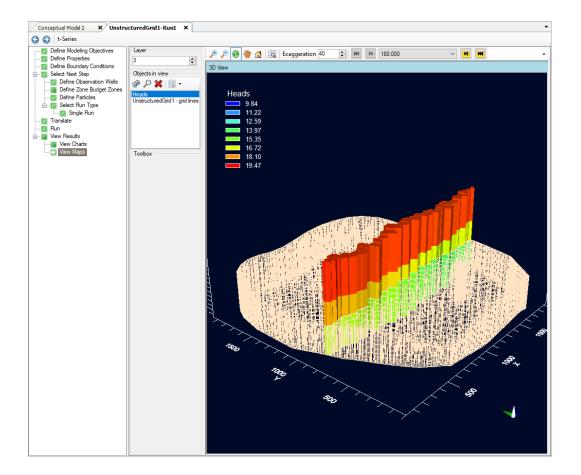
- By default the view is plan (from above); take a moment to rotate the view as previously described, and apply the desired vertical exaggeration (40 is a good setting for this example). The default option is to the selected layer as a slice. You can display heads along a specific layer, or cross-section by adjusting the settings.
- Right-click on 'Heads' from the Model Explorer (under 'Run1/Output/Flow'), and select [Settings] from the pop-up menu:



 Next from the 'Settings' tree on the left, expand 'Slice', turn on the check box beside 'Show Slice', and change the Slice Type to 'Row'. You will also change the 'XZ Slice Position' to '50'. This indicates that a cross-section will be displayed in the X direction, including all cells which intersect the desired location. The XZ slice position value is expressed as a percentage of the entire distance in the selected direction.

· General · Style	General	
• Style • Cells	✓ Show Slice	
🗄 - Lines	Slice Settings	
	Slice Type AutoApply	
···· General	Row	~
···· Colors ···· Legend	XZ Slice Position (min=1, max=100)	50
⊞ · Color Map ⊞ · Time		
	Fill Settings By Attribute Transparency 0	Show Cell ID Jahele
	By Attribute Transparency 0	Show Cell ID labels
	By Attribute Transparency	÷

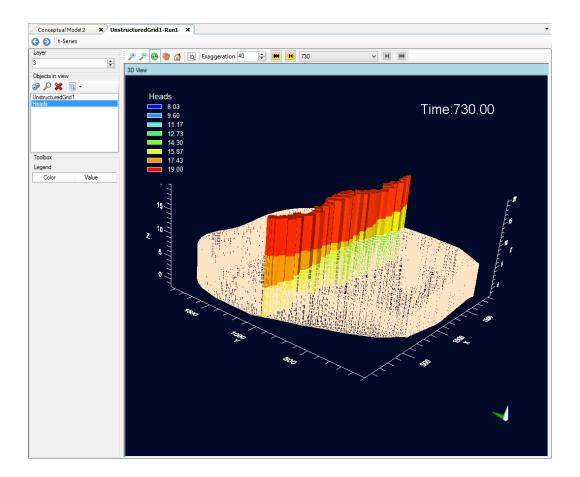
- Click the **[OK]** button to apply these changes to the 3D View, and close the **'Settings'** window.
- You should then see cells rendered along the X direction, approximately half-way through the model domain, as shown below:



Please Note: changing the displayed layer using the menu at the top left may cause changes to the slice settings. If this does happen simply reset the slice to its original position in the Settings window.

- For Transient models, the 3D Displays can be updated to display calculated heads (or drawdown) from different time steps. Use the time-step picker menu above the 3D viewer to choose from the available time-steps. Additional options for time steps are located in the 'Settings'.
- Repeat the same steps above to load the 'Settings' window. Expand 'Style', and select the 'Time' node from the tree, and you should see the following display:

- In the 'Settings' window, activate the ' Show time label' checkbox
- In the main window, above the 3D View, you should see a **'Time-Step Picker'** menu, which lists available output times. Choose the desired output time from this list and the 3D View will update with the calculated heads from that time step. Take a moment to experiment with these options.
- If you select the final time step, the resulting view should look like the following image:



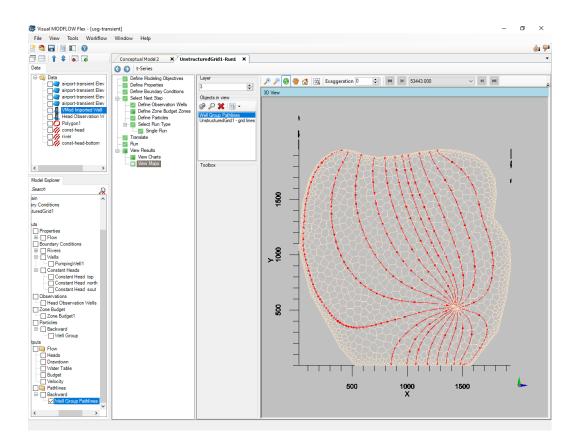
Export

The calculated heads and drawdown can be exported to a (point or polygon) shapefile or to a text file (.CSV), for further post-processing. This option is available by right-clicking on the **'Heads'** item on the Model Explorer, and selecting **[Export...]**. The heads can be exported to either point or polygon shapefiles, with attributes. This option is not covered in this Tutorial exercise.

View Maps (Pathlines)

Displaying particle pathlines is very easily done. Reset the 3D viewer window to its original state by clicking the 'Reset View' button, then activate the pathline outputs from the Model Explorer.

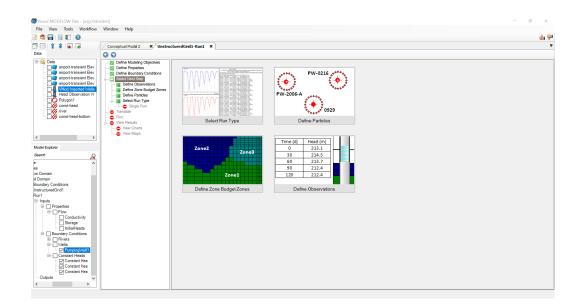
- Click the [1] (Reset View) button in the 3D viewer toolbar
- Uncheck Heads under the Model Explorer, to hide the output heads
- **Well Group Pathlines** under the Model Explorer, to display the particle pathlines
- You should then see the backward tracking particles that we had placed around the pumping wells, as shown below:



View Charts Step: Viewing Model Chart Data

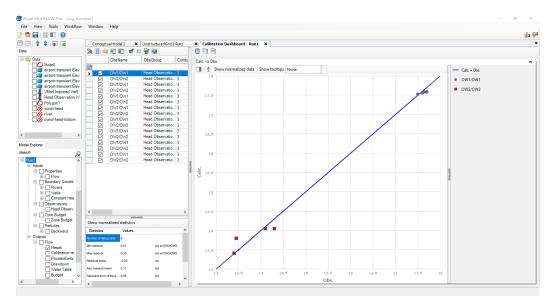
In this section you will learn how to compare the observed concentration data to the concentration values calculated by the model.

- Select the [View Charts] item from the workflow tree, under 'View Results'
- Click [Open Dashboard] to proceed.



As you can see from the image below, Visual MODFLOW Flex supports a number of methods for selecting different wells. It will always be possible to turn on/off wells in particular layers.

• Take a moment to view the correlation between calculated and observed heads



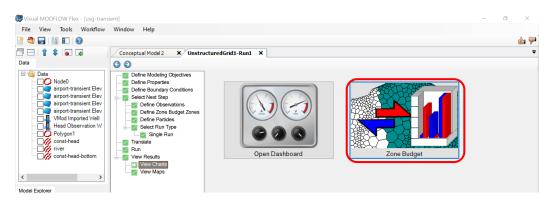
You can change the chart type to display 'Time Series' graph, and see the corresponding charts for the desired observation points.

- Click 'Chart selector' [
- Then, under 'Chart selector' select 'Time Series' and deselect 'CalcVsObs'

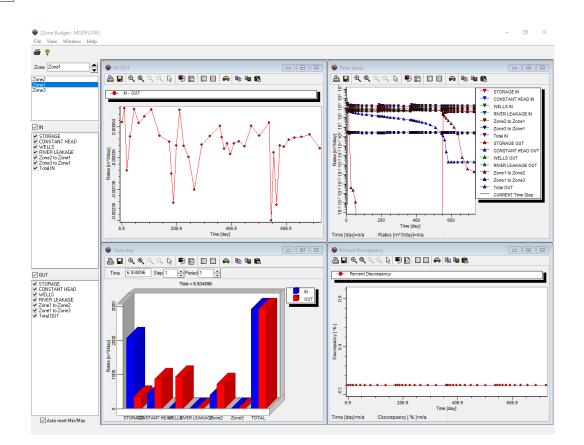
View Tools Workflow	Window	Help									
3 🔚 🔢 🗊 🙆											da 9
3 1 1 1 🕡 🖓	Conceptua	I Model 2 🗙	UnstructuredGrid1	-Run1	× Calibration Dasht	oard - Run1 ×					
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👔 Data		ObsName	ObsGroup	Condu							
Node0		Obsiname	Obstaroup	Condu	Time Series						
- airport-transient Elev		OW1/OW1	Head Observatio		📑 🍦 Show norm	alized data Show tooltips	None				- OW1/OW1-(Row) Cal
- airport-transient Elev		0\w2/0\w2	Head Observatio.		18						
irport-transient Elev		OW2/0W2	Head Observatio								 OW1/OW1-(Row) Ob
airport-transient Elev		OW2/OW2	Head Observatio			•					- OW2/OW2-(Row) Cal
- VMod Imported Well		OW2/OW2 OW1/OW1	Head Observatio		17.5						
Head Observation W		0W2/0W2	Head Observatio								OW2/OW2-(Row) Ob
Polygon1		OW1/OW1	Head Observatio								
river		OW2/OW2	Head Observatio								
const-head-bottom		OW1/OW1	Head Observatio		17						
		0\v/2/0\v/2	Head Observatio.								
		0\v1/0\v1	Head Observatio	3							
>		0\v/2/0\v/2	Head Observatio	3	16.5						
xplorer		O\w1/O\w1	Head Observatio.								
	M	0\v/2/0\v/2	Head Observatio	3							
2		OW1/OW1	Head Observatio.		16						
un1 A	M	0\v/2/0\v/2	Head Observatio.	3							
- Inputs					2						
Properties					÷						1
Flow					[ш] 15.5 Н						
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E Zone Budget	<			>	14.5						
Zone Budget		-									
Particles	Show norma	lized statistics									
Backward	Statistics	Values		^	14						
Outputs	Residual mean	-0.02	(m)								
Flow	Abs, residual mea	n 0.11	(m)								
Heads					13.5						
Calibration re	Standard error of		(m)								
FloodedCells Drawdown	Root mean square	id 0.16	(m)								
Water Table	Noramized rootm	ean 3.74	(%)		13						
Budget y	Correlation coeffic				13 0	100 200	300	400 500	600	700 800	
V	Commentation country			~				Time			< >

View Zone Budget Results

To review the results of the ZoneBudget analysis simply click the **'Zone Budget'** button located at the 'View Charts' workflow step:

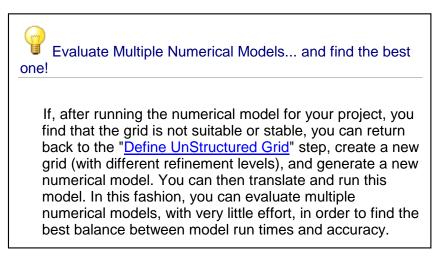


• You should see the following window open (the four sub-windows have been rearranged to better display the contents of the Zone Budget window):



Zone budget analyses are an easy way for you to better understand the water budget in areas of interest within your model.

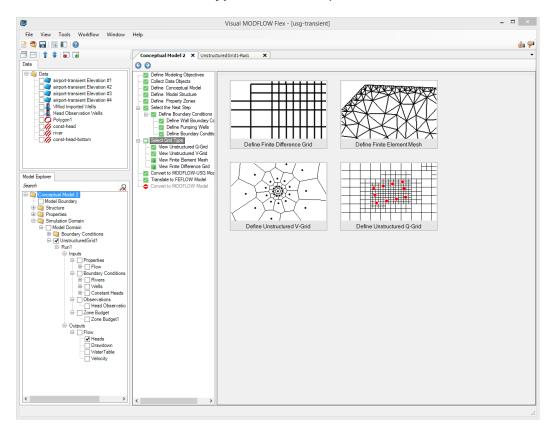
 Once you have reviewed the Zone Budget results you may close the Zone Budget window



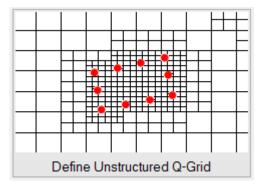
Defining Unstructured Q-Grids

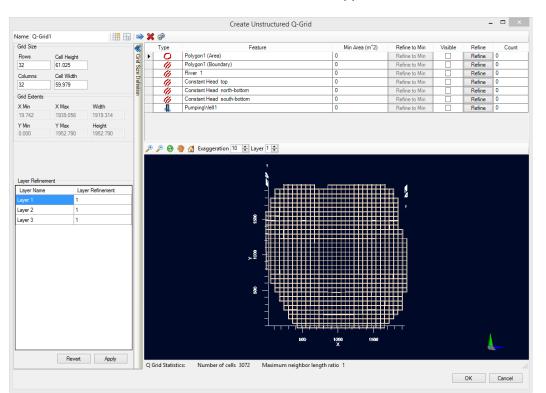
The conceptual modeling workflow allows the user to test a variety of different grid types very quickly and easily. In this section we will return to the conceptual model to generate a new unstructured grid type (quadtree grid or Q-grid), merge the conceptual model and Q-grid into a single MODFLOW-USG numerical model and re-run the model.

- At the top of the grid view you will see a list of active tabs. Click the 'Conceptual Model 2' tab to return to the conceptual modeling workflow.
- Return to the 'Select Grid Type' workflow step, as shown below



- This time we will select the 'Define Unstructured Q-Grid' option
- Click the 'Define Unstructured Q-Grid' button





• The 'Create Unstructured Q-Grid' window will appear, as shown below:

The 'Create Unstructured Q-Grid' window includes a list of the data objects which have been used to define model elements (e.g. polyline, polygon, and/or point data objects used to define boundary conditions). Using the 'Refine' and 'Refine to Min' buttons in the table allow you to perform successive refinements around the selected data object. The 'Refine' button will split the cells that intersect with the selected data object into four smaller equally sized cells. The 'Refine to Min' button will perform successive refinements until a given minimum area threshold (user defined, in the 'Min Area' column) is reached. Experiment with these options and perform some refinements around the pumping well, river and constant head boundary objects.

- Click the 'Refine' button in the 'PumpingWell1' row twice (x2)
- Click the 'Refine' button in the 'River 1' row once (x1)
- Type '500' in the 'Min Area (m^2)' field for the 'Polygon1 (Boundary)' data object
- Click the 'Refine to Min' button in the 'Polygon1 (Boundary)' row
- When you're finished the **'Create Unstructured Q-Grid'** window should look like the image below (note the refined grid cells around the selected data objects; also note that the **'count'** column tracks the number of refinements performed for each data object):

					Create Unstructured Q-Grid					
lame Q-Grid	2	🏥 E	-	💥 🖗 📈						
Grid Size				Туре	Feature	Min Area (m^2)	Refine to Min	Visible	Refine	Count
Rows	Cell Height		G	0	Polygon1 (Area)	0	Refine to Min		Refine	0
32	61.025		Grid Size Definition	· (1)	Polygon1 (Boundary)	500	Refine to Min		Refine	1
Columns	Cell Width		Ze	4	River 1	0	Refine to Min	-	Refine	1
32	59.979		Defi	11	Constant Head top	0	Refine to Min		Refine	0
	00.070		litio	4	Constant Head north-bottom	0	Refine to Min		Refine	0
Grid Extents			- 1	14	Constant Head south-bottom	0	Refine to Min		Refine	0
X Min	X Max	Width		4	PumpingWell1	0	Refine to Min	-	Refine	2
19.742	1939.056	1919.314								
Y Min	Y Max	Height								
0.000	1952.790	1952.790								
Layer 3					8 _					
	1				80 T 1					
	Revert	Apply			8	+				

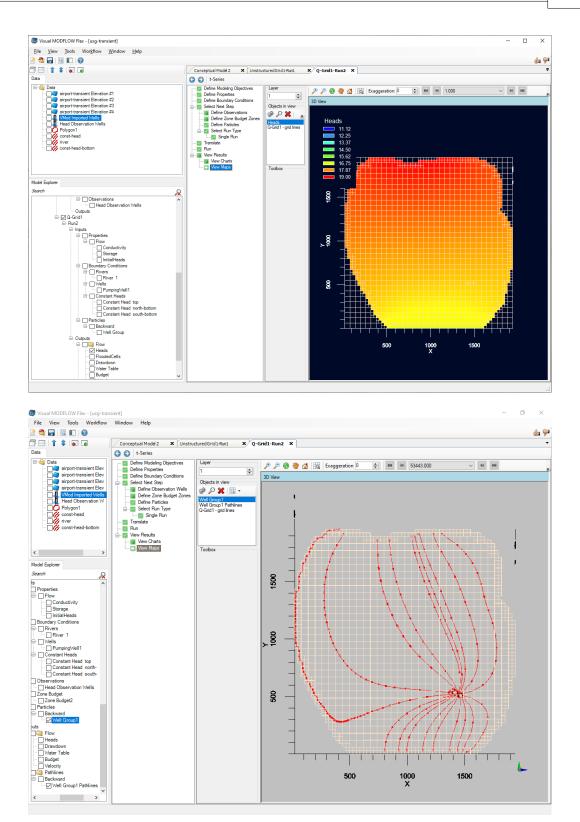
Click OK

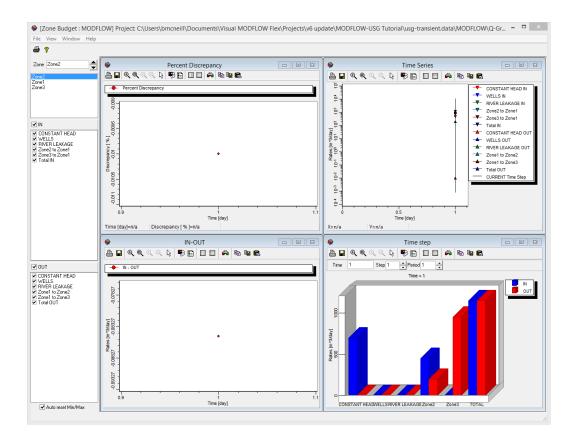
The unstructured Q-grid is now available for the conceptual to numerical model conversion. Follow the same steps as above to convert the conceptual model to a numerical model, review properties and boundary conditions, apply zone budget zones and/or particles, and finally translate and run the unstructured Q-grid model. The only exceptions are the following:

• When defining the particles, select a Radius of 20 m and 12 particles per circle:

			- 🗆	×
Particle group nam	le	Particle propagation		
Well Group1		Forward Sackward		
Select object		Release time End time O Beginning of simulation		
	ported Wells	End of simulation		
Particles on circle		Custom		
Radius: (m)	20	0		
# Particles	12			
Particles along scr	een			
# Circles				
	L			
	L			

Once you have completed these steps you should see results similar to the following images displaying head distributions, particle pathlines and zone budget results, respectively. (note: results are displayed for a steady-state simulation):



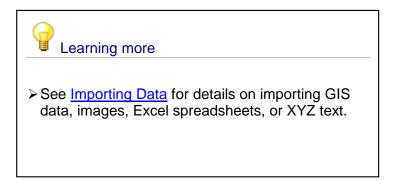


*****This concludes the 'Groundwater Flow Modeling with MODFLOW-USG' tutorial.*****

4 Working with Your Data

The modeling workflows in Visual MODFLOW Flex are data driven. This means that you first need to load or create the appropriate data objects in order to use these at a particular step in the workflow. See the following table for some common examples:

If you have	First you should	Then you can
River locations in a shapefile	Import these as <u>Polyline</u> data objects	Select this data object when creating a river boundary condition
Geological layers in a Surfer .GRD or ASCII GRD	Import these as <u>Surface</u> data objects	Select these data objects when defining horizons
Aerial photo with river locations	Import this as a <u>Map</u> image Then <u>Create a new</u> <u>Polyline</u> data object Digitize the polyline in a 2D Viewer	Select this new polyline data object when creating a river boundary condition
XYZ points for geological contacts	Import these as <u>Points</u> data objects Then "Create Surfaces" from these data objects	Select these surfaces when defining horizons or numerical model layers
Raster Grid of Kx or Recharge data (from Surfer, ESRI .GRD)	Import these as surface data objects	Select these data objects when defining properties or Recharge boundary conditions
Visual MODFLOW (Classic) project or USGS MODFLOW files	Select the Numerical model workflow after creating a project	Select these files when prompted to Import Model. <u>Learn more</u>



- See <u>Creating Data Objects</u> for more details on digitizing new point, polygon, or polyline data object.
- See <u>Creating Surfaces</u> for more details on interpolating XYZ data to be used as geological layers or 2D parameter distributions.

4.1 Importing Data

Visual MODFLOW Flex supports importing data from various standard data types to allow you flexibility in constructing your model. Data can be imported and used in several ways; spatial data can be used to delineate and visualize geometry of structural zones, horizons and features of your conceptual model, while attribute data can be used in assigning properties to structural zones and attributes to boundary conditions.

Getting Started

You can start the import process by any of the following methods:

- Select File > Data Import from the main menu
- Press CTRL + D
- Right-click in the Data Explorer and select Import Data... from the pop-up menu.

The data import process in Visual MODFLOW Flex varies slightly depending on the data type being imported. However, the import process generally consists of the following steps:

- 1. Select the data type and source file
- 2. Specify the coordinate system (including projection and datum) of the source data
- 3. Map the source data fields with required target fields, and map attribute fields
- 4. Data preview and validation

Supported File Types

The following sections provide additional information on the import process for each data type:

- Points
- Image: Market Polylines
- O Polygons

- 🖺 <u>Wells</u>
- Image: Surfaces
- I <u>3D Gridded Data</u>
- MGA Cross-Sections
- <u>Time Schedules</u>
- <u>Maps</u> and <u>DXFs</u>

Imported data will be <u>validated</u> to verify that data records can be imported. If import errors are encountered, you will be prompted to decide how to handle these errors.

4.1.1 Points

Points represent discrete locations in space (XYZ) where attribute information is known. Examples of points data include: ground surface or subsurface elevations, well tops, locations with known aquifer hydraulic properties, etc. Typically, this information may come from drilling wells or monitoring events where information is gathered from a specific location.

Once imported, points data can then be interpolated to generate surfaces. These surfaces can be used to create conceptual model horizons, or for defining property values for structural zones. For more information on creating surfaces from points data see <u>Creating</u> <u>Surfaces</u>.

Visual MODFLOW Flex supports the following file types for points data:

- Shapefile (*.SHP)
- AutoCAD (*.DXF)
- Text (*.TXT)
- Comma-Separated Values (*.CSV)
- Access Database (*.MDB)
- Excel (*.XLS)

For Points data, the following data must exist in separate columns, in your source data:

- X
- Y
- Elevation
- Attribute 1 (optional) (e.g., conductivity)
- Attribute 2 (optional) (e.g., layer 2 elevation)
- etc..

To import points data, follow the steps below:

• Right-click in the Data Explorer, and select Import Data... from the pop-up menu. The import dialog will open:

	Data Import			-	
Data Source					
Data Type: *					
Point					~
Source File: *					
Name: *					
Description:					
		< <back< td=""><td>Next >> (</td><td>Cancel</td><td>Help</td></back<>	Next >> (Cancel	Help

Select Points from the Data Type drop-down list. Click the [...] button and locate the source file.

Enter a Name and a Description (optional) for the imported data, and click [Next] to continue.

• The next step allows you to preview the source data before importing, and will vary depending on which file type is selected.

For .CSV and .TXT files (shown below), select the appropriate delimiter from the Delimiters frame, e.g., if it is a *.CSV file, you would select "comma". Specify which row to start importing from using the From row selector.

🔜 Data Import			<u>_ ×</u>
Delimiters Space Tab Other:	Comma	From row	
Preview Source Data			
	Row	Column1	
1		mw-4,740,1612,1,178.31,1,183.55	
2		mw-6,895,1295,1,176.66,1,183.48	
3		mw-7,905,754,1,177.61,1,183.03	
4		mw-8,885,814,1,177.27,1,183.1	—µ
5		mw-10,1170,1210,1,183.18,1,183.45	
6		mw-11,1132,1611,1,179.83,1,183.65	
7		mw-13,1192,585,1,176.72,1,182.9	
8		mw-15,835,1095,1,177.39,1,183.36	
9		mw-19,885,1335,1,176.57,1,183.49	
10		mw-20,885,1395,1,176.48,1,183.51	
11		mw-21,877,1487,1,176.94,1,183.55	
12		mw-22,873,1529,1,175.56,1,183.57	
13		mw-23,1007,1449,1,165.54,1,183.56	
1.4		04 1010 1000 1 170 04 1 100 00	_
		< Back Next >> Cancel Help	

For .XLS files (shown below), select which Excel worksheet to import from the Select Worksheet drop down list. Also, you can choose which row to import from using the From row selector.

l	Sheet1\$				•	From 1	-				
	eview Source Dat										
10	Row	×	Y	Z	lay2	lay3	lay4	WellName	Kx (ft/day)	Initial Heads	-
1	1	574366.6799	4862849.399	21	11	7	2	1	20.3	16	
	2	574366.6799	4862900	19.1	12.1	8.1	-1	2	18.1	14.1	-
ł	3	574366.6799	4863050	21.2	11.2	7.2	-1	3	20.3	16.2	-
2	4	574366.6799	4863349.399	20.3	13.3	7.3	1	4	19.5	15.3	-
	5	574520	4863349.399	18.1	12.1	8.1	0.1	5	18.3	13.1	-
7	6	574666	4862849.399	20.3	9	11	1.3	6	19.5	15.3	
7	7	574666	4863000	18.1	9.5	10.5	2.1	7	18.3	13.1	
ì	8	574666	4863349.399	20.3	13.3	6.3	0.3	8	19.5	15.3	
P	9	574720	4862849.399	19.5	11.5	7.5	1.5	9	17	14.5	
7	10	574800	4863050	18.3	10.3	8.3	0.3	10	11	13.3	
2	11	574850	4862849.399	19.5	12.5	6.5	-2	11	13.5	14.5	
2	12	574850	4862999	18.3	11.3	8	0.3	12	11	13.3	٦
7	13	574850	4863050	19.5	10.5	7.5	1.5	13	13.5	14.5	
2	14	574850	4863349.399	17	11	8	-1	14	11	12	
2	15	574900	4863120	16.5	13.5	8.5	1.5	15	11	11.5	

For .MDB files (shown below), you can choose to import data from a table or a query, by selecting either the View Tables or View Queries radio button. Select the desired query/table from the Select Table or Query drop down list box.

Borehole	3			T	 View T View G 				
Preview Sou	irce Data								_
Row	ID	×	Y	Z	Layer2	Name	Layer3	Layer4	
9 1	1	536212.689999	4814029.99999	2323.5	2623.5	GB-01	2823.5	3123.5	
9 2	2	536156.69	4814049.99999	2326	2626	GB-02	2826	3126	
9 3	3	536079.69	4814069.99999	2326	2626	GB-03	2826	3126	
9 4	4	535953.69	4814019.99999	2322	2622	GB-04	2822	3122	
7 5	5	535848.689999	4814059.99999	2324	2624	GB-05	2824	3124	
76	6	535743.689999	4814069.99999	2330.5	2630.5	GB-06	2830.5	3130.5	
97	7	535652.69	4814029.99999	2333	2633	GB-07	2833	3133	
7 8	8	535498.69	4814039.99999	2329.5	2629.5	GB-08	2829.5	3129.5	
7 9	9	535386.69	4814059.99999	2329.5	2629.5	GB-09	2829.5	3129.5	
7 10	10	535295.69	4814029.99999	2338	2638	GB-10	2838	3138	
7 11	11	535232.69	4813999.99999	2339.5	2639.5	GB-11	2839.5	3139.5	
7 12	12	536225.92	4814281.79999	2325.93	2625.93	GB-12	2825.93	3125.93	
7 13	13	536129.740000	4814379.69999	2324.85	2624.85	GB-13	2824.85	3124.85	
7 14	14	536065.76	4814320.19999	2323.05	2623.05	GB-14	2823.05	3123.05	
/ 15	15	535960.34	4814251.29999	2324.26	2624.26	GB-15	2824.26	3124.26	
7 16	16	535866.679999	4814349.39999	2326.56	2626.56	GB-16	2826.56	3126.56	

Next, select the Coordinate System of the data being imported. If the coordinate system is different than the one defined in the project settings, VMOD Flex will perform a geo-transformation, converting all coordinates to the project's coordinate system. Click the [Next>>] button to continue to the next step.

Geographic information for the source data	
Coordinate Systems: *	
UTM Zone 17N(WGS84)	
Datum: *	
World Geodetic System 1984	
Local Coodinate System	
	< Back Next >> Cancel Help

Next, set your Data Mapping by mapping columns in the source data to the target fields in Visual MODFLOW Flex. A read-only preview of the source data is presented. The process of data mapping is described in the following section in greater detail.

	elds	Map_to		Unit category		Unit	Multiplier		Data type
×	×		Length		m	1		Numerio	
Y	Y		Length	1	m	1		Numerio	
Elevation	N	one	None		None	1		Numerio	
Þ 🗙									
urce Data Previ	ew								
urce Data Previ X	ew Y	Z	lay2	lay3	lay4	WellName	Kx (ft/day)	Initial Heads	
× 574366.6799	Y 4862849.399	21	11	7	2	1	20.3	16	
× 574366.6799	Y		11 12.1	7 8.1	-				
	Y 4862849.399	21	11 12.1 11.2	7 8.1 7.2	2	1	20.3	16	
× 574366.6799 574366.6799	Y 4862849.399 4862900	21 19.1 21.2 20.3	11 12.1 11.2 13.3	7 8.1 7.2 7.3	2	1 2	20.3 18.1 20.3 19.5	16 14.1 16.2 15.3	
× 574366.6799 574366.6799 574366.6799	Y 4862849.399 4862900 4863050	21 19.1 21.2	11 12.1 11.2	7 8.1 7.2 7.3 8.1	2 -1 -1	1 2 3 4 5	20.3 18.1 20.3	16 14.1 16.2 15.3 13.1	
× 574366.6799 574366.6799 574366.6799 574366.6799 574520	Y 4862849.399 4862900 4863050 4863349.399	21 19.1 21.2 20.3	11 12.1 11.2 13.3	7 8.1 7.2 7.3	2 -1 -1 1	1 2 3 4	20.3 18.1 20.3 19.5	16 14.1 16.2 15.3	-
× 574366.6799 574366.6799 574366.6799 574366.6799	Y 4862849.399 4862900 4863050 4863349.399 4863349.399	21 19.1 21.2 20.3 18.1	11 12.1 11.2 13.3 12.1	7 8.1 7.2 7.3 8.1	2 -1 -1 1 0.1	1 2 3 4 5	20.3 18.1 20.3 19.5 18.3	16 14.1 16.2 15.3 13.1	
× 574366.6799 574366.6799 574366.6799 574366.6799 574520 574666	Y 4862849.399 4862900 4863050 4863349.399 4863349.399 4862849.399	21 19.1 21.2 20.3 18.1 20.3	11 12.1 11.2 13.3 12.1 9	7 8.1 7.2 7.3 8.1 11	2 -1 -1 1 0.1 1.3	1 2 3 4 5 6	20.3 18.1 20.3 19.5 18.3 19.5	16 14.1 16.2 15.3 13.1 15.3	

Data Mapping

The first column in the Data Mapping table, named **Target_Fields**, contains the required target fields for the data object. The second column, named **Map_to**, allows you to match the fields in the source data to each required target field.

If the column labels in the source data are identical to the labels of the target fields, Visual MODFLOW Flex will automatically map the columns for you. However, if the labels differ, you must map the columns manually.

To map a source field to a target field, select the corresponding source field from the drop list box in the Map_to column. The drop down list displays the column headers in the data source file.

Target_ fields	Map_to	Unit category	Unit	Multiplier	Data type
X	X	Length	m	1	Numeric
Y	Y	Length	m	1	Numeric
Elevation	None	▼ None	None	1	Numeric
	Z lay2 lay3 lay4 WellName				

For example, in the figure above, the elevation field in the source data is labeled "Z". To map this field to the target field "Elevation", select "Z" from the adjacent drop down list.

If the file you are trying to import is a 3D Shapefile (with Elevation defined), then Visual MODFLOW Flex should automatically detect this, and you should not need to map the Elevation attribute at this step. You can also specify a data field as the source of elevation information, if appropriate.

Adding Attributes

Source fields that are not required, can be mapped by creating a new attribute. To create a new attribute, click the Add a new attribute button. A new row will be added to the Data Mapping table.

Data Mapping					
Target_ fields	Map_to	Unit category	Unit	Multiplier	Data type
X	X	Length	m	1	Numeric
Y	Y	Length	m	1	Numeric
Elevation	Z	Length	m	1	Numeric
Create a new attribute	None	▼ None	None	1	Numeric
<u>+</u> ×	Y Z lay2 lay3 lay4 WellName Kx (ft/day) Initial Heads				

In the Map_to column, select the desired attribute field in the source data, from the combo box. Repeat for additional attributes. You can delete a mapped attribute by selecting the row

from the Data Mapping table, and then clicking the \Join Delete button.

Use the Unit Category and Unit columns to define the units of a mapped field. If the specified units are different than those defined in the Project Settings, Visual MODFLOW Flex will automatically convert the data in the source file to the default project units.

The Multiplier column allows you to multiply all values in the mapped field by a specified multiplier value.

The Data Type column allows you to define the data type. Select from the following options: Numeric, Text, Boolean, Date and Time. For example, if the mapped column contains text data, select Text from the drop down list.

Once the data mapping is complete, click the [Next] button to continue to the validation step.

4.1.2 Polylines

Polyline data consists of a series of points (vertices) connected by lines. Polyline data objects can be used in Visual MODFLOW Flex for defining geometry and assigning attributes to linear boundary conditions, such as River and Drain boundary conditions.

Polylines may also be useful to visualizing geographic features such as river and road networks.

Visual MODFLOW Flex supports the following file types for polyline data.

- Shapefile, *.SHP
- AutoCAD, *.DXF

To import polyline data, follow the steps below:

- Right-click in the Data Explorer, and select Import Data... from the pop-up menu.
- Select Polyline from the Data Type drop down list.
- Click the [...] button and locate the source file.
- Enter a Name and a Description and then click [Next] to continue.

The next step involves selecting the coordinate system of the source file, and will vary depending on which file-type is selected for the source file.

For .SHP files, if the associated .PRJ file is located in the same location as the source file, Visual MODFLOW Flex can automatically detect the coordinate system of the source data and will perform a geotransformation if the coordinate system is different than that defined in the project settings. If a .PRJ file is missing, than you will be prompted to select the Coordinate System for the data being imported.

For .DXF files, you will always be prompted to select the Coordinate System of the selected source file.

Click the [Next] button to continue.

If the file type is .SHP, the next step involves creating attributes. If you are importing from .DXF file, you can skip this step.

			Data	Import			
ata	Mapping						
1.	Target fields	Map to	Unit category	Unit	Multiplier	Data Type	
X		X	Length	m	1	Numeric	
Y		Y	Length	m	1	Numeric	
E	levation	Elevation	Length	m	1	Numeric	
_							
ł	• 🗙						
our	ce Data Preview						
ur	rce Data Preview						
ur	rce Data Preview						
ur	rce Data Preview						
ur	rce Data Preview						
ur	rce Data Preview						
ur	ce Data Preview						
ur	ce Data Preview						
ur	ce Data Preview						
ur	ce Data Preview						
ur	ce Data Preview						>

If the file you are trying to import is a 3D Shapefile (with Elevation defined), then Visual MODFLOW Flex should automatically detect this, and you should not need to map the Elevation attribute at this step. You can also specify an attribute field as the source of elevation information. For example, if you have contour information.

This dialog allows you to import shapefile attributes. To create a new attribute, click the Add a new attribute button. When selected, a new row will be added to the Data Mapping table.

In the Map_to column, select the desired attribute field in the source data, from the combo box. Repeat for additional attributes. You can delete a mapped attribute by selecting the row from the Data Mapping table, and then clicking the Delete button.

For a description of the Unit Category, Unit, Multiplier and Data Type columns, please refer to section "<u>Data Mapping</u>" section.

Click the [Next] button to continue.

The final step involves validation of the data being imported. This step will ensure that the data set contains valid data for each of the mapped columns.

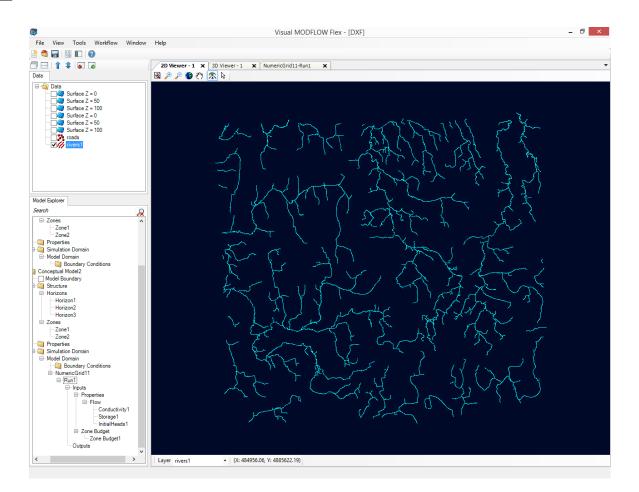
For .SHP files, please refer to "<u>Data Validation</u>" section for more information on the data validation step.

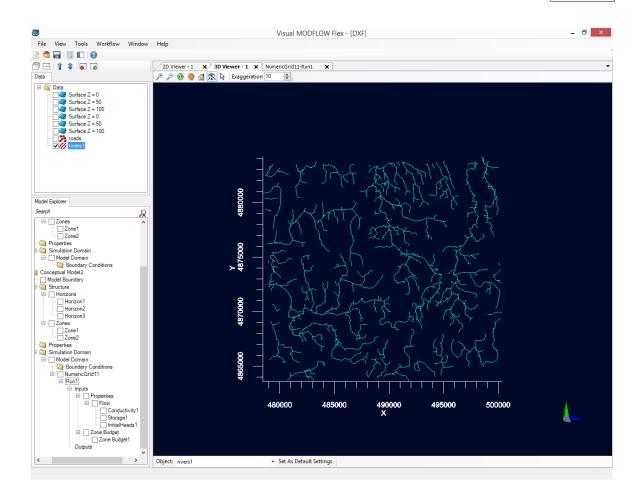
For .DXF files, the following dialog will show, indicating the number of polylines that will be created from the source file.

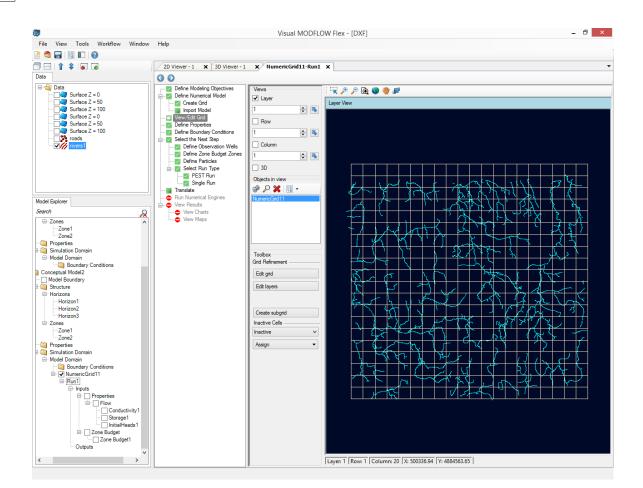
🔜 Data Import	
Number of DXF entities processed: 1	
Number of Polylines created: 2	
	< Back Cancel Help

Click the [Finish] button to complete the polygon importing process. Once imported, a polyline data object will be added to the Data Explorer.

You can visualize your polyline data objects by displaying them in a 2D or 3D Viewer or the Layer View within the Numerical Workflow. For example a DXF of the rivers:







You can adjust the Style settings for the DXF in each of the viewers. For more information on adjusting please review <u>Points</u>, <u>Polylines</u>, <u>and Polygons</u> section.

4.1.3 Polygons

Polygons are closed shapes consisting of vertices, line segments and have at least 3 sides. Polygons can be used in Visual MODFLOW Flex in the following ways:

- To define the horizontal boundary of a conceptual model
- To define the geometry and attributes of horizontal boundary conditions, e.g., recharge, specified-head.
- To define the geometry and attributes of property zones.
- To visualize spatial variation of geographic features using various style settings.
- Visual MODFLOW Flex supports the following file types for polygon data.

The following polygon file types are supported:

- Shapefile, *.SHP
- AutoCAD, *.DXF

To import polygon data, follow the steps below:

- Right-click in the Data Explorer and select Import Data... from the pop-up menu.
- Select Polygon from the Data Type drop down list box.
- Click the [...] button and locate the source file.
- Enter a Name and a Description for the imported data, and click [Next] to continue.

The remaining workflow for importing polygon data is very similar to that of importing Polylines. For more information on how to import polygons, please see <u>Importing Polylines</u>

4.1.4 Wells

Wells are natively conceptualized in Visual MODFLOW Flex via Well objects. A well object contains a list of wells that are represented within it and various levels of associated detail, including the following types of information:

- Well Name,
- Location (separate x/y coordinate fields),
- Top Elevation,
- Well Bottom (as depth or elevation),
- (non-vertical) well path,
- depth intervals of screen(s),
- pumping schedule,
- parameters for well/formation hydraulics,
- head or concentration observations,
- · target heads or concentration observations, and/or
- hydrostratigraphic layer thicknesses

Well objects can be created within Flex or imported from tabulated information and the following file types are supported for well data:

- Comma-Separated Values (*.CSV)
- Excel (*.XLS, *.XLSX)

At a minimum, the imported file must contain the fields denoted above in bold. Other fields may be required based on the type of information to be imported, as described below. Once imported, wells data can be used to build well boundary conditions and/or observations.

Starting the Import Process

To import wells, start the general import wizard by:

- Right-clicking in the Data Explorer and select Import Data... from the pop-up menu,
- Selecting File > Data Import from the main menu, or
- Pressing CTRL + D

Once, the wizard has opened:

- Select Wells from the Data Type drop down list.
- Click the [...] button and locate the source file.
- Enter a Name and a Description for the imported data, and click [Next] to continue.

Initial Data Preview

The second step allows you to preview the source data before importing, and choose a subset of the source data, e.g., a worksheet, data range, or named table within an excel file.

 If the data to be imported is in an Excel file, select the desired data range to import from the Select Worksheet drop-down list. Also, you can choose which row to import from using the From Row text field.

Select Worksheet	t			From rov	v			
Import-Pumping\$			~	1	* *			
eview Source Dat	a							
Well ID	X	Y	Elevation	Well Bottom	Screen ID	Screen Bottom Z	Screen Top Z	
Well-A	6250	46250	500	0	1	0	500	
PW-01	13750	46250	500	50	1	50	500	Τ
PW-02	21250	46250	500	50	1	50	500	T
Well-B	28750	46250	500	0	1	0	500	
PW-03	6250	38750	500	50	1	50	500	T
PW-04	13750	38750	500	50	1	50	500	1
PW-05	21250	38750	500	50	1	50	500	1
PW-06	28750	38750	500	50	1	50	500	1
PW-07	6250	31250	500	50	1	50	500	1
PW-08	13750	31250	500	50	1	50	500	1
PW-09	21250	31250	500	50	1	50	500	+
PW-10	28750	31250	500	50	1	50	500	1
PW-11	21250	16250	500	0	1	0	50	1
Simple-C	16250	21250	500	0	1	0	50	1
PW-12	8750	8750	500	50	1	50	500	+
			1	1		1		>

• If the data to be imported is in a CSV file, you will be prompted to select the field delimiter(s) and the row where the data starts:

Delimiters Space Tab Other:		Comma	1	n row	i name		
eview Source Data	Well ID	×	Y	Elevation	Well Bottom	Screen ID	Screen Top Z
1	Well-A	6250	46250	500	0	1	500
2	PW-01	13750	46250	500	50	1	500
3	PW-02	21250	46250	500	50	1	500
4	Well-B	28750	46250	500	0	1	500
5	PW-03	6250	38750	500	50	1	500
6	PW-04	13750	38750	500	50	1	500
7	PW-05	21250	38750	500	50	1	500
8	PW-06	28750	38750	500	50	1	500
9	PW-07	6250	31250	500	50	1	500
10	PW-08	13750	31250	500	50	1	500
11	PW-09	21250	31250	500	50	1	500
12	PW-10	28750	31250	500	50	1	500
13	PW-11	21250	16250	500	0	1	50
/	1	1		1	1	1	-

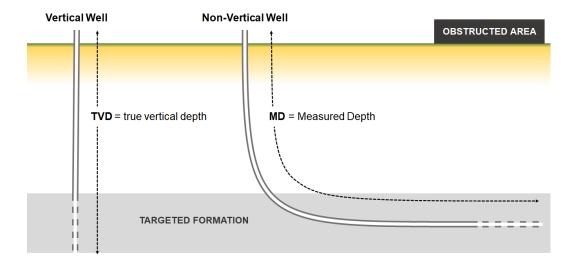
Selecting the Well Information Type(s)

At the third step in the well import process, Visual MODFLOW Flex provides you three groups of options for importing wells and associated well data:

🝔 Data Import			_		\times
Select the format of the vertic	al data in your data so	ce			
Non-vertical Wells	Elevation	O Measured depths			
Time					
Absolute					
◯ Relative					
Select the type of data you w	ant to import				
Well heads only with Id, >	, y, Elevation and dep	1			
O Well heads with the follow	ving data				
 Screens (ID, location 	s)				
Pumping sched	ule Well Mod	WEL ~			
 Observation points 					
Observed head	s				
Observed conc	entrations				
Target residuals	3				
 Well tops 					
		< <back next="">></back>	Cancel	He	lp 🛛

Vertical reference and alignment

This section is used to specify the vertical alignment of the well and the type of vertical positioning data that will be used for the well object.



Non-vertical Wells checkbox: To import non-vertical wells (also known as horizontal or deviated wells), select the "Non-vertical Wells" checkbox; otherwise leave the box unchecked.

Depth Type (Elevation or Measure Depth): The depth type is used to specify how the vertical data is expressed in the source file. If the data is expressed with respect to a vertical reference datum, e.g., above mean sea level, then select Elevation. If the vertical data is expressed as a depth, e.g., distance from ground to the bottom of the well, then select Measured Depth. The measured depth option is automatically required if importing non-vertical wells and will require additional data in the form of x,y,z coordinate triplets along the entire path of the well bore as opposed to the simpler format of x,y pairs and top/bottom elevation information for a vertical well bore.

Please Note: You can import and manage multiple well objects (also known as well groups) in your project, so it may make sense to import non-vertical wells separately from vertical wells as the data requirements are somewhat different for each. See below how to map non-vertical wells in the Data Mapping section.

Time Options

If time-varying data is to be imported for a pumping schedule or observed values, the specified times can be imported as Absolute (e.g. calendar date 5/15/2020) or Relative times (e.g. 1 day, 30 days, 365 days, etc), where the value is relative to the start time defined in the Modeling Objectives for the first conceptual or numerical model present in the Modeling Tree.

Data Type

There are two general types of well information supported:

Well Heads Only: is the option to import just the well heads, i.e., X-Y coordinates, elevation, and well depth for each well. Use this option if you have limited data about your wells and/or will be adding the data later.

Well Heads with the Following Data: is the option to import additional data for each well. Options include:

<u>Screens</u> (ID/Location): Import the screen locations for each well. You can also optionally select the Pumping Schedule check box to import pumping schedules for each screen. This data could be used later to define pumping well boundary conditions. Furthermore, you can also select one of the supported well models, including: WEL, MNW1, or MNW2.

<u>Observation Points</u>: Import observation points for each well. Select either Observed heads or Observed Concentrations. You may also import target residual values by selecting the checkbox.

<u>Well tops</u>: Import the elevation (or measured depth) of points along the well path, where geologic formation (contact points) intersect with the well. This data could be used later to generate surface and horizon layers.

Please Note: For data requirements for each option, please see the next step "Data Mapping".

Once you have selected which well data to import, click the [Next] button to proceed to the data mapping.

Data Mapping

This step requires you to map the columns in the source data to the required target fields. The required fields will vary depending on the type of well data you selected in the previous step. The following sections describe the data mapping for each data type option:

Well Heads Only

For importing Well Heads only, you must map the following columns from the source data to the required target fields (denoted by a red asterisk):

- Well ID: a unique value in the source data. If not, any rows containing duplicate Well IDs will be skipped and not imported.
- X: the x-coordinate of the well
- **Y**: the y-coordinate of the well
- Elevation: the elevation/depth of the well head, and
- Bottom: the bottom elevation/depth of the well borehole

To map a target field, click on the corresponding entry in the Map to column and select the appropriate column from the source data using the dropdown menu that will appear. Source Data fields with names that match a target field will be mapped automatically. An example is shown below:

		Ta	rget fields		Map to		Unit cate	egory		Unit	Multiplier	Da	ta Type	
٦	•	Well Id		We	II ID		None		None		1	Text		_
	ŀ	X		X			Length		m		1	Numeric		_
	ŀ	Y		Y			Length		m		1	Numeric		-
	ŀ	Elevation		Ele	vation		Length		m		1	Numeric		-
	ŀ	Well bottom	1	We	II Bottom	\sim	Length		m		1	Numeric		_
	-			row	ı	~			1		1			-
٩e	equ	uired		КЪ										
L		N/2		X										
╞		×		Y	vation									
		> Data Preview	/	Y Ele	vation Il Bottom	¥		4		4		1		
ur	rce	Well ID	row	Y Ele	Il Bottom col	~	Kt		Къ	×	Y		levation	
our	rce	Well ID ell-A	row 3	Y Ele	Il Bottom col 3	-	1	2	Къ	6250	46250	500	evation	
	rce We PV	Well ID ell-A V-01	70W 3 3 3	Y Ele	Il Bottom col 3 6	-	1	1	Кь	6250 13750	46250	500 500	levation	
	rce We PV	Well ID ell-A V-01 V-02	row 3	Y Ele	Il Bottom col 3 6 9	-	1	1	Къ	6250 13750 21250	46250 46250 46250	500 500 500	levation	
	rce We PV	Well ID ell-A V-01 V-02 ell-B	row 3 3 3 3 3 3	Y Ele	Il Bottom col 3 6 9 12		1	1	Къ	6250 13750 21250 28750	46250 46250 46250 46250	500 500 500 500	levation	
	rce We PV	Well ID ell-A V-01 V-02	row 3 3 3 3 3 6	Y Ele	Il Bottom col 3 6 9 12 3		1 1 1	1 1 2 1	Къ	6250 13750 21250 28750 6250	46250 46250 46250	500 500 500 500 500	levation	
	rce We PV PV PV	Well ID ell-A v-01 v-02 ell-B v/-03 v/-04	row 3 3 3 3 6 6 6	Y Ele	Il Bottom col 3 6 9 12 3 6		1 1 1 1 1 1 1	1 1 2 1 1	Kb	6250 13750 21250 28750 6250 13750	46250 46250 46250 46250 38750 38750	500 500 500 500 500 500 500	levation	
	rce We PV PV PV	Well ID ell-A v-01 v-02 ell-B v-03	row 3 3 3 3 3 6	Y Ele	Il Bottom col 3 6 9 12 3		1 1 1 1 1 1	1 1 2 1	Kb	6250 13750 21250 28750 6250	46250 46250 46250 46250 38750	500 500 500 500 500	levation	

Wells Heads with Screens

If this option is selected, you must first map the well heads under the Well Heads tab (as shown in the section above). Next, click on the Screens tab, and map the appropriate columns from the source data to the following target fields:

	Target fields	Map to	Unit category	Unit	Multiplier	Data Type
•	Screen Id	Screen ID	None	None	1	Text
•	Screen top Z	Screen Top Z	Length	m	1	Numeric
•	Screen bottom Z	Screen Bottom Z	Length	m	1	Numeric

- Screen ID: unique ID for the well screen
- Screen top Z: elevation/depth of top of screen
- Screen bottom Z: elevation/depth of bottom of screen

For each well in the source data, the Screen ID must be unique. Also, screens should not overlap within a single well. These requirements will be validated in the final step of the well import process.

Well Heads with Screens and a Pumping Schedule (WEL Model)

If you selected the pumping schedule check box in the previous step, click the Pumping Schedule tab and then map the appropriate columns from the source field to the following target fields:

	Target fields	Map to	Unit category	Unit	Multiplier	Data Type
•	Pumping start date	None	None	None	1	DateTime
•	Pumping end date	None	None	None	1	DateTime
•	Pumping rate	Pumping Rate	Pumping Rate	m^3/d	1	Numeric

- **Pumping Start Date**: in MM/DD/YYYY HH:MM:SS format or relative time as a numeric value in the chosen units.
- **Pumping End Date**: in MM/DD/YYYY HH:MM:SS format or relative time as a numeric value in the chosen units.
- Pumping Rate: the pumping rate for the current scheduled interval

Please Note: If time is not included in the source data (just the date), Visual MODFLOW Flex will automatically set the time to 12:00:00 am.

Well Heads with Screens and a Pumping Schedule (MNW1 Model)

If you selected the MNW1 well model in the previous step, the Pumping Schedule tab will have additional optional fields that can be mapped based on the input dataset. If the optional fields are not mapped at this step, default values will be added to the do not need to be mapped and then map the appropriate columns from the source field to the following target fields:

Target fields	Map to	Unit category	Unit	Multiplier	Data Type
Pumping start date	None	None	None	1	DateTime
Pumping end date	None	None	None	1	DateTime
Pumping rate	Pumping Rate	Pumping Rate	m^3/d	1	Numeric
Rw	Rw	Length	m	1	Numeric
RSkin	Rskin	Length	m	1	Numeric
KSkin	None	Conductivity	m/d	1	Numeric
В	None	None	None	1	Numeric
С	None	None	None	1	Numeric
CWC	None	None	None	1	Numeric
CWCDistribution	None	None	None	1	Text
WaterLimit	WaterLimit	None	None	1	Numeric
QCUT	QCUT	None	None	1	Numeric
Hlim	Hlim	Length	m	1	Numeric
Href	Href	Length	m	1	Numeric
Qfrcmn	Qfrcmn	None	None	1	Numeric
Qfrcmx	Qfrcmx	None	None	1	Numeric

Well heads Screens Pump Schedule

- **Rw**: Radius of the well screen (L)
- RSkin: Radius of the well skin (L)
- KSkin: Hydraulic conductivity of the well skin (L/T)
- B: Linear well loss coefficient
- C: Non-linear well loss coefficient
- CWC: cell to well loss coefficient
- CWC Distribution: Option for defining how the CWC coefficient is apportioned across the cell(s) spanning the screen (ByCell, By Screen Thickness, By Cell Transmissivity)
- WaterLimit: Option to set the reference type for HLim and Href
 - "Water Level": water level constraints are based on the absolute water level in the specified well
 - "Drawdown": water level contraints are based on relative water level in the specified well (drawdown)
- **HLim:** limiting water level in the well (a minimum for discharging wells [Q<0] and a maximum for injection wells [Q>0]. For example, if the head in the well falls below this value in a discharging well, then pumping in the well ceases.
- **Href**: Reference elevation for the limiting water level (HLIM). If the value of HREF is greater than the maximum water level at the beginning of stress period 1, HREF is set to the simulated water level at the location of the head/drawdown-limited well.
- **QCut**: Option to set pumping rate limit types for Qfrcmn and Qfrcmx
 - Qfrcmn: Pumping rate or fraction (see QCUT) below which pumping will cease
 - Qfrcmx: Pumping rate or fraction (see QCUT) above which pumping will resume/be reactivated

Well Heads with Screens and a Pumping Schedule (MNW2 Model)

If you selected the MNW2 well model in the previous step, the Well Heads tab will have additional optional fields that can be mapped based on the input dataset. If the optional fields are not mapped at this step, default values will be added to the do not need to be mapped and then map the appropriate columns from the source field to the following target fields:

	Target fields	Map to	Unit category	Unit	Multiplier	Data Type
Ŀ	Well Id	Well ID	None	None	1	Text
Ŀ	X	X	Length	m	1	Numeric
ŀ	Y	Y	Length	m	1	Numeric
ŀ	Elevation	Elevation	Length	m	1	Numeric
ŀ	Well bottom	Well Bottom	Length	m	1	Numeric
	LossType	None	None	None	1	Text
	P	None	None	None	1	Numeric
	Rw	Rw	Length	m	1	Numeric
	RSkin	Rskin	Length	m	1	Numeric
	KSkin	None	Conductivity	m/d	1	Numeric
	В	None	None	None	1	Numeric
	С	None	None	None	1	Numeric
	CWC	None	None	None	1	Numeric
	CWCDistribution	None	None	None	1	Text

- LossType: Options for MNW2
 - \circ NONE
 - \circ THIEM
 - o SKIN
 - o LINEAR
 - NONLINEAR
 - SpecifyCWC
- Rw: Radius of the well screen (L)
- RSkin: Radius of the well skin (L)
- KSkin: Hydraulic conductivity of the well skin (L/T)
- B: Linear well loss coefficient
- C: Non-linear well loss coefficient
- CWC: cell to well loss coefficient
- **CWC Distribution**: Option for defining how the CWC coefficient is apportioned across the cell(s) spanning the screen (ByCell, By Screen Thickness, By Cell Transmissivity)
- WaterLimit: Option to set the reference type for HLim and Href
 - "Water Level": water level constraints are based on the absolute water level in the specified well
 - "Drawdown": water level contraints are based on relative water level in the specified well (drawdown)
- **HLim:** limiting water level in the well (a minimum for discharging wells [Q<0] and a maximum for injection wells [Q>0]. For example, if the head in the well falls below this value in a discharging well, then pumping in the well ceases.
- **Href**: Reference elevation for the limiting water level (HLIM). If the value of HREF is greater than the maximum water level at the beginning of stress period 1, HREF is set to the simulated water level at the location of the head/drawdown-limited well.
- **QCut**: Option to set pumping rate limit types for Qfrcmn and Qfrcmx:
 - $\circ\,$ "None": there is not a minimum pumping rate below which the pump becomes inactive
 - o "Rate": the pumping limits are specified as a rate (L3/T)
 - o "Percent": the pumping limits are specified as percentage of the pumping rate Qdes
- Qfrcmn: Pumping rate or fraction (see QCUT) below which pumping will cease

Qfrcmx: Pumping rate or fraction (see QCUT) above which pumping will resume/be reactivated

If you selected the MNW2 well model in the previous step, the Pump Schedule will have additional optional fields that can be mapped based on the input dataset:

		Target fields	Map to	Unit category	Unit	Multiplier	Data Type
	•	Pumping start date	None	None	None	1	DateTime
	•	Pumping end date	None	None	None	1	DateTime
	•	Pumping rate	Pumping Rate	Pumping Rate	m^3/d	1	Numeric
		QCUT	QCUT	None	None	1	Numeric
		Hlim	Hlim	Length	m	1	Numeric
		Qfrcmn	Qfrcmn	None	None	1	Numeric
Þ		Qfrcmx	Qfrcmx	None	None	1	Numeric

- **HLim:** limiting water level in the well (a minimum for discharging wells [Q<0] and a maximum for injection wells [Q>0]. For example, if the head in the well falls below this value in a discharging well, then pumping in the well ceases.
- **QCut**: Option to set pumping rate limit types for Qfrcmn and Qfrcmx:
 - "None": there is not a minimum pumping rate below which the pump becomes inactive
 - o "Rate": the pumping limits are specified as a rate (L3/T)
 - o "Percent": the pumping limits are specified as percentage of the pumping rate Qdes
- Qfrcmn: Pumping rate or fraction (see QCUT) below which pumping will cease
- Qfrcmx: Pumping rate or fraction (see QCUT) above which pumping will resume/be reactivated

Well Heads with Observation Points

When this option is selected, you must first map the well heads under the Well Heads tab (described above). Next, click the Observation Points tab, and map the appropriate columns from the source data to the following target fields:

Observed Heads:

		Target fields	Map to	Unit category	Unit	Multiplier	Data Type
	•	Obs.Point Id	Logger_Id	None	None	1	Text
	•	Obs.Point Z	Logger_Z	Length	m	1	Numeric
	•	Observed Head	Observed_Head	Length	m	1	Numeric
	•	Head observation date	None	None	None	1	DateTime
Þ	•	Target Residual	None	Length	m	1	Numeric

- Obs Point ID: a label that is unique for its parent well identifying an observation point within a given well
- Obs Point Z (Elevation/depth): elevation/depth of the observation point
- **Observed Head:** the measured head in the observation well in units of length (feet or meters)
- **Target Residual**: the acceptable modeling error for heads (used for calibration/history matching) in units of length (feet or meters)
- Head Observation Date: the date/time of the observation

Observed Concentrations:

		Target fields	Map to Unit category		Unit	Multiplier	Data Type
	•	Obs.Point Id	Logger_Id	None	None	1	Text
	•	Obs.Point Z	Logger_Z	Length	m	1	Numeric
	•	Chemical	None	None	None	1	Text
	•	Concentration	None	Concentration	mg/L	1	Numeric
	•	Concentration observation da	None	None	None	1	DateTime
Þ	•	Target Residual	None	Concentration	mg/L	1	Numeric

- **Obs Point ID:** a label that is unique for its parent well identifying an observation point within a given well
- Obs Point Z (Elevation/depth): elevation/depth of the observation point
- **Chemical:** the name of the chemical constituent that was measured (which must exactly match the species name in the Modeling Objectives)
- Observed Concentration: the measured/observed concentration at the observation point
- Concentration Observation Date: the date/time the observation was measured
- **Target Residual**: the acceptable modeling error for concentrations (used for calibration/history matching)

The Obs. Point Z (Elevation) will determine in which model layer (cell) the observed head/concentration was measured; at the time when you view charts, Visual MODFLOW Flex will find the calculated head value from the same cell, and then use this for comparing your observed value to what MODFLOW calculated. The same is true for Transport runs, but in this case it will take concentration from that cell, and compare to what you observed in the field.

Well Heads with Well Tops

When this option is selected, you must first map the well heads under the Well Heads tab (described above). Next, click on the Tops tab and map the appropriate columns from the source data to the following target fields:

- Top Z: elevation (or measured depth) of formation
- Top ID: formation name, e.g., Sand1, Sand2, Clay etc.

Wel	he	ads Tops						
	Target fields		Map to Unit category		Unit	Multiplier	Data Type	
	•	Top Id	None	None	None	1	Text	
F	•	Top Z	None	Length	h m		Numeric	
					·		·	

Please Note: the well top data in the source file must be formatted as follows:

		Тор Z				
well ID	Top ID	(elevation-based)	(depth-based)			
Well1	Fill	52	0			
Well1	Sand1	26	26			
Well1	Clay	6.5	45.5			
Well2	Fill	94	0			
Well2	Sand1	17	77			
Well2	Clay	4	90			

Non-Vertical Wells

When the Non-Vertical Wells option is selected at the Well Information step, you must map the 3D well path information (instead of the Well Head) under the Well Path tab, as well as any other applicable data tabs (described above):

		Target fields	Map to	Unit category	Unit	Multiplier	Data Type
	•	Well Id	Well_Name	None	None	1	Text
	•	X	X-world_coord(m)	Length	m	1	Numeric
	•	Y	Y-world_coord(m)	Length	m	1	Numeric
Þ	•	Elevation	Elevation(m)	Length	m	1	Numeric

- Well ID: a unique value for each distinct well that must be repeated for each X,Y,Z coordinate triplet that describes the well path.
- X: the x-coordinate of a point along the well path
- Y: the y-coordinate of a point along the well path, and
- Elevation: the absolute elevation of a point along the well path

Please Note: related objects along this path in other the other import tabs such as well screens and observation points must be expressed in terms of the measured depth along the well path.

Validation Step

The final step in the Well import process is data validation. Visual MODFLOW Flex will validate the mapped data, and highlights any rows that contain invalid data, e.g., null values, wrong assigned data type, duplicate rows etc.

	a Import							—		\times
	nd warnings									
🚫 Hea	ads 📀 Screer	ns 📀 Pump Sch	edule							
		al								
Do r	not import rows w	th warnings								
Mapped	Data Preview									
	Screens Pum	p Schedule								
	Row	Well Id	х	Y	Elevation	Well bottom	Errors			~
<i>I</i> 1		Well1	490250	4876150	313	280				
J 2		Well2	490150	4876250	317	279		-		
		1		-1	1	1		1		
										~
<										>
						< <b< td=""><td>ack Finish</td><td>Cancel</td><td>He</td><td>In</td></b<>	ack Finish	Cancel	He	In
							THISIT	Cancel	TIE	P

Please see "Data Validation" section for more information on data validation.

Click the [Next] button to import the data. Once imported, a Wells data object will be added in the Data Explorer.

4.1.5 Surfaces

Surface data consists of an ordered array of interpolated values at regularly spaced intervals that represent the spatial distribution of an attribute, e.g., digital elevation models. Surface data can be used in Visual MODFLOW Flex in the following ways:

- To define the horizons (the interface between structural zones) of a conceptual model.
- To define the spatial distribution of a boundary condition attribute (e.g. recharge, evapotranspiration).
- To define the spatial distribution of a property zone attribute (e.g., conductivity, initial heads).

• To visualize the spatial variation of model features, (e.g. surface topography, water table elevation, etc.)

Visual MODFLOW Flex supports the following surface file types:

- SURFER Grid Files (*.GRD)
- ESRI ASCII Raster Files (*.ASC, *.TXT)
- USGS Digital Elevation Model (*.DEM)

Import Steps

Surfaces are imported using the Import Data wizard. To access the wizard, follow the steps below:

- Right-click in the Data Explorer and select **Import Data...** from the pop-up context menu,
- Press [CRTL]-D, or
- Select File > Import Data from the Main Menu

Step 1 - File Selection

The first step in the surface import is to specify the location and type of file to imported:

- Select Surface from the Data Type drop down list box.
- Click the [...] button and locate the source file.
- Enter a Name and a Description for the imported data, and click [Next] to continue.

🐯 Data Import	_		×
Data Source			
Data Type: *			
Surface			\sim
Source File: *			
C:\Users\Public\Documents\Visual MODFLOW Flex\Tutorials\Conceptual Model\supp files\ground.GRD			
Name: *			
ground			
Description:			
< <back next="">> Ca</back>	ncel	He	In
	1001	ine	P

Please Note: Surface files that contain a large quantity of data points may require substantial time to import into Visual MODFLOW Flex.

Step 2 - Coordinate System Selection

Next, select the Coordinate System of the data being imported. If the coordinate system is different than the one defined in the <u>project settings</u>, Visual MODFLOW Flex will perform a geotransformation, converting all coordinates to the project's coordinate system. Note that the options provided at this step will be disabled if the project uses a local coordinate system, since the local coordinate system will not have a basis for coordinate conversions.

🐡 Data Import —		×
Geographic information for the source data		
Coordinate Systems: *		
SPCS83 Virginia Southern Zone(ft)		\sim
Datum: *		
NORTH AMERICAN 1983, CONUS		
Local Coodinate System		
< <back <u="">Next >> Cancel</back>	Hel	р

Click the [Next] button to continue to the next step.

Step 3 - Data Mapping

Supported surface data formats only consist of three columns: X, Y and elevation/attribute data. Although surfaces imported into Visual MODFLOW Flex most often represent actual surfaces with elevations such as ground surface or the elevations at the interface between model layers, surfaces can also represent other distributed data (e.g. conductivities, concentrations, recharge, etc) as described above. Visual MODFLOW Flex will automatically map the source columns to the target fields; however if your surface represents other data or the data are not based in project units, you can use the Unit category and Unit fields to specify units for the data. If the data are associated with units other than the project units, the data will be converted from the specified units into the project units.

The lower portion of the window at this step provides a preview of the mapped data before importing into Visual MODFLOW Flex:

	Mapping		4	4	4	4	4
		Target fields	Map to	Unit category	Unit	Multiplier	Data Type
•	X		X	Length	ft	1	Numeric
-	Y		Y	Length	ft	1	Numeric
•	Elevation	l .	Elevation	Length	ft	1	Numeric
ł	uired						
ourc	e Data Pre X	view	Elevation				
1 1/	000	-1500	612.4885604				
	120	-1500	612.8784576				
_							
1	240	-1500	613.3581658				
11		-1500 -1500	613.3581658 613.9583914				
1 12 13	240						
11 12 13 14	240 360	-1500	613.9583914				
11 12 13 14 16	240 360 480	-1500 -1500	613.9583914 614.7112865 615.6393648 616.7441291				
11 12 13 14 10 10	240 360 480 600	-1500 -1500 -1500	613.9583914 614.7112865 615.6393648				

Click the [Next] button to finish the import process.

Step 4 - Validation

The final step in the import process is validation - Visual MODFLOW Flex will inspect the data to be imported and reports any errors with the data that it finds. You can also preview a portion of the data using the "*show this amount*" option.

🐯 Data Import				-		×
No errors or warnings were found						
Do not import rows with warnings Mapped Data Preview 7950 records were mapped						
Show only errors and warmings	Show this amount Apply	100				
Row X Y Elevation	n Errors					^
<		< <back< td=""><td><u>F</u>inish</td><td>Cancel</td><td>Help</td><td>> ~</td></back<>	<u>F</u> inish	Cancel	Help	> ~

To import the surface data, click the [Finish] button.

Upon importing, a new data object will be added to the Data Explorer.

4.1.5.1 SURFER Grid Files

Visual MODFLOW Flex supports the import of SURFER ASCII Grid Files (*.grd).

Format

The format of a Surfer ASCII grid file consists of six items:

```
DSAA
Nx Ny
Xmin Xmax
Ymin Ymax
Zmin Zmax
Zl Z2 Z3 Z4 ... Znx
Znx+1 ...
. .
```

... Znx*ny

Where:

Parameter	Description
DSAA key	first line of the file must include the text "DSAA" which is a text key used to indicate that the file is a SURFER ASCII grid file
Nx Ny	Nx - the number of grid cells in the x-direction (integer) Ny - the number of grid cells in the y-direction (integer)
Xmin Xmax	Xmin - the X-coordinate in the left-/western-most cell Xmax - the X-coordinate in the right-/eastern-most cell
Ymin Ymax	Ymin - the Y-coordinate in the bottom-/southern-most cell Ymax - the Y-coordinate in the top-/northern-most cell
Zmin Zmax	Zmin - the smallest value in the surface Zmax - the largest value in the surface

Data Block See description below

Data Block

The data component of the SURFER ASCII grid follows the header information.

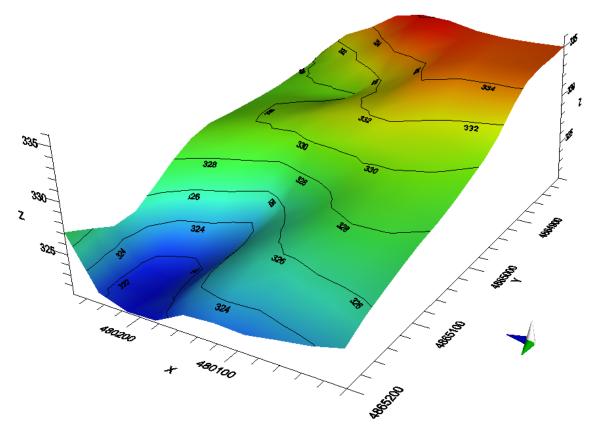
- Cell values should be delimited by spaces.
- No carriage returns are necessary at the end of each row in the raster.
- Row 1 of the data is at the bottom (south) side of the raster, row 2 is the data for the next northward data above row 1, and so on.

Example

An example dataset follows:

```
DSAA
10 15
480000 480275
4864800 4865200
321.162 336.095
335.007 334.943 334.974 335.267 335.899 336.095 335.553
333.868 332.647 330.317
```

334.818 334.729 334.820 335.349 335.765 335.623 333.998 332.027 330.824 329.693 334.743 334.640 334.695 335.157 334.620 334.012 332.142 330.947 330.267 329.528 334.337 334.291 334.323 334.729 333.095 331.948 329.890 329.682 329.606 329.314 333.094 333.228 333.393 333.985 332.567 331.600 330.137 329.879 329.704 329.278 331.413 331.859 332.229 332.919 332.253 331.781 330.973 330.326 329.915 329.304 330.267 331.006 331.457 331.975 331.785 331.566 330.869 330.279 329.891 329.355 329.510 330.272 330.688 330.975 330.612 330.271 329.539 329.721 329.755 329.496 328.748 329.396 329.695 329.593 328.536 327.843 326.796 327.963 328.638 329.024 328.164 328.715 328.879 328.422 326.930 325.949 324.327 325.862 326.817 327.945 327.754 328.045 328.072 327.573 326.338 325.279 322.970 323.706 324.460 326.505 327.139 327.053 326.932 326.492 325.839 325.008 322.361 321.909 322.297 325.212 326.452 326.145 325.915 325.448 325.291 324.766 322.293 321.339 321.549 325.050 325.728 325.247 324.908 324.425 324.513 324.136 322.078 321.162 321.638 326.150 324.672 323.889 323.423 322.897 323.037 322.829 321.355 321.259 322.214 327.178



Imported example dataset, as displayed in Visual MODFLOW Flex.

4.1.5.2 ESRI ASCII Raster Files

Visual MODFLOW Flex supports the import of ESRI ASCII Raster Files (*.asc).

Format

The format of an ESRI ASCII raster file consists of seven items:

NCOLS XXX NROWS XXX XLLCORNER XXX YLLCORNER XXX CELLSIZE XXX NODATA_VALUE XXX Z1 Z2 Z3 Z4 ... Znx Znx+1 Znx*ny

Where:

Parameter	Description	Requirements
NCOLS	Number of cell columns.	Integer greater than 0.
NROWS	Number of cell rows.	Integer greater than 0.
XLLCORNE R	X coordinate of the origin (lower left corner of the cell).	
YLLCORNER	Y coordinate of the origin (lower left corner of the cell).	
CELLSIZE	Cell size.	Greater than 0.
NODATA_V ALUE	The input values to be NoData in the output raster.	Optional. Default is -9999.
DATA BLOCK	See description bel	ow

Data Block

The data component of the ESRI ASCII raster follows the header information.

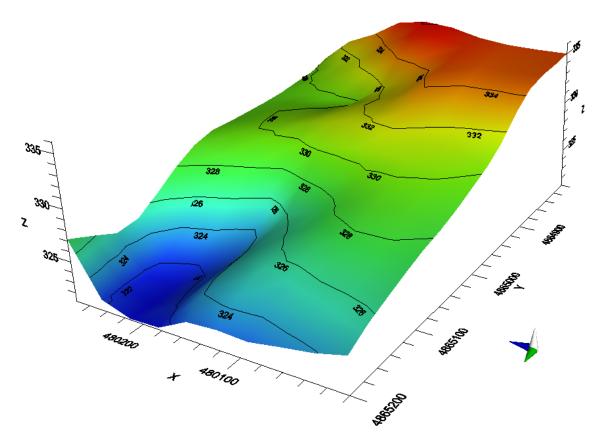
- Cell values should be delimited by spaces.
- No carriage returns are strictly necessary at the end of each row in the raster. The number of columns in the header determines when a new row begins.
- Row 1 of the data is at the top (north) side of the raster, row 2 is the data for the next southward data below row 1, and so on.

Example

An example dataset follows:

```
NCOLS 10
NROWS 15
XLLCORNER 480000
YLLCORNER 4864775
CELLSIZE 25
NODATA_VALUE -999
324.672 323.889 323.423 322.897 323.037 322.829 321.355
321.259 322.214 327.178
325.728 325.247 324.908 324.425 324.513 324.136 322.078
321.162 321.638 326.150
326.452 326.145 325.915 325.448 325.291 324.766 322.293
321.339 321.549 325.050
```

327.139 327.053 326.932 326.492 325.839 325.008 322.361 321.909 322.297 325.212 327.754 328.045 328.072 327.573 326.338 325.279 322.970 323.706 324.460 326.505 328.164 328.715 328.879 328.422 326.930 325.949 324.327 325.862 326.817 327.945 328.748 329.396 329.695 329.593 328.536 327.843 326.796 327.963 328.638 329.024 329.510 330.272 330.688 330.975 330.612 330.271 329.539 329.721 329.755 329.496 330.267 331.006 331.457 331.975 331.785 331.566 330.869 330.279 329.891 329.355 331.413 331.859 332.229 332.919 332.253 331.781 330.973 330.326 329.915 329.304 333.094 333.228 333.393 333.985 332.567 331.600 330.137 329.879 329.704 329.278 334.337 334.291 334.323 334.729 333.095 331.948 329.890 329.682 329.606 329.314 334.743 334.640 334.695 335.157 334.620 334.012 332.142 330.947 330.267 329.528 334.818 334.729 334.820 335.349 335.765 335.623 333.998 332.027 330.824 329.693 335.007 334.943 334.974 335.267 335.899 336.095 335.553 333.868 332.647 330.317



Imported example dataset, as displayed in Visual MODFLOW Flex.

4.1.6 3D Gridded Data

3D Gridded Data refers to 3D grids with attributes assigned to each grid cell. 3D Gridded data can be used in VMOD Flex to visualize heads generated from a MODFLOW run in Visual MODFLOW Flex, or for assigning spatially-variable attributes to boundary conditions and property zones. Visual MODFLOW Flex supports the following file types for 3D Gridded data:

- MODFLOW Heads file,*.HDS
- MT3D/RT3D/SEAWAT/MODFLOW-SURFACT Concentration File, *.UCN
- TecPlot 3D Point Grid File, *.DAT

Please Note: In order to import data from .HDS and/or .UCN files, the source file must exist in the folder that contains all associated MODFLOW data files, e.g., .DIS, .NAM etc.

To import 3D Gridded data, follow the steps below:

- Right-click in the Data Explorer and select Import Data... from the pop-up menu.
- Select 3D Gridded Data from the Data Type drop down list.
- Click the [...] button and locate the source file.
- Enter a Name and a Description for the imported data, and click [Next] to continue.
- Next, select the Coordinate System of the 3D Gridded data. If the coordinate system is different than the one defined in the project settings, VMOD Flex will perform a geotransformation, converting all coordinates to the project's coordinate system. Click the [Next] button to continue to the next step.

The next step allows you to specify how the gridded data is to be imported.

😻 Data Import	_		×
Import Settings Import the true grid dimensions. High quality, slower performance. Import a reduced grid size. Lower quality, higher performance. The true grid data can be retrieved from the data object after import Import every 1 + th node Select Existing Grid			
Numerical grid object you want to assign the data to			
< <back next="">></back>	Cancel	Help	

When importing a .HDS or .UCN file, the Gridded data for existing grid option will be automatically selected. The grid dimensions in the source file must be identical to the dimensions of a grid in your project. Select the existing numerical grid from Conceptual Model tree, and then click the button.

When importing a .DAT file, the Gridded data for existing grid option will be not be available. When this option is selected, the Grid Origin frame will display. If the gridded data is in model coordinates, specify the Grid Origin and the degree of Rotation. If the grid is in world coordinates, you may leave the grid origin as is.

Data Import		-		\times
Import Settings Import the true grid dimensions. High quality, slower performance. Import a reduced grid size. Lower quality, higher performance. The true grid data can be retrieved from the data object after import Import every 1 I				
	< <back ne<="" td=""><td>ext >> Cancel</td><td>He</td><td>p</td></back>	ext >> Cancel	He	p

For both file types, you can specify the grid resolution. To import the full grid dimensions, select Import the true grid dimensions option.

Please Note: Depending on the performance capabilities of your computer, 3D Gridded data containing large volumes of data may take a significant time to import.

To improve importing and viewing performance, select the Import a reduced grid size option, and specify a value in the Import every nth node box. For example, if a value of 2 is defined, then VMOD Flex will only import every other node in the 3D grid.

Next, select the appropriate Data Category, Unit, and Data Type for each of the mapped attributes.

OT INC	s definition Target fields	Map to	Unit category	Unit	Data Type
X		X	Length	m	Numeric
Y		Y	Length	m	Numeric
E	Elevation	Z	Length	m	Numeric
12	Z"	"Z"	Length	m	Numeric
1	'KX"	"KX"	Conductivity	m/d	Numeric
1	'KY"	"KY"	Conductivity	m/d	Numeric
1	"KZ"	"KZ"	Conductivity	m/d	V Numeric

The final dialog in the import process for 3D Gridded shows the grid dimensions of the source data.

😂 Data Import			_		\times
Source dimension Number of rows:	Number of layers				
Number of columns:	Number of time steps				
Cell top elevation attribute					
		< <back finis<="" td=""><td>h Cancel</td><td>He</td><td>elp</td></back>	h Cancel	He	elp

The Source Dimensions frame displays the Number of Rows, Number of Layers, Number of Columns and Number of Time Steps in the source data.

Finally, click the [Finish] button to import the 3D Gridded data.

4.1.6.1 TecPlot 3D Point Grid File

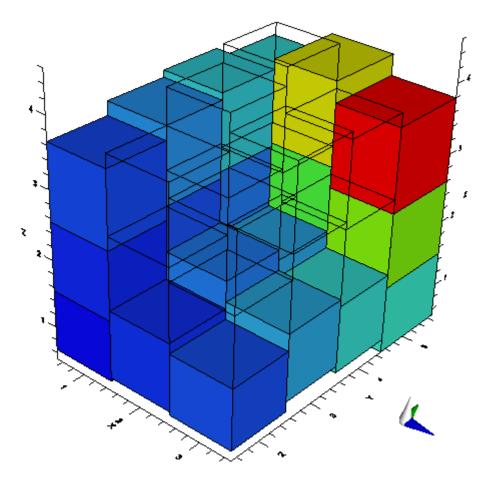
Visual MODFLOW Flex supports the import of 3D-gridded data in the TecPlot ASCII IJK-Ordered data point format (*.dat). The format consists of four items:

- 1. TITLE used to specify a brief description of the dataset, must be enclosed in quotes
- VARIABLES used to specify the data variables encoded in the IJK-Ordered input, values must be enclosed in quotes and separated by commas and the values must start with "X", "Y", "Z", followed by any number of spatially distributed data variables
- 3. **ZONE** used to specify the indices of the IJK data and the format:
 - I is the number of columns along the X-direction
 - J is the number of rows along the Y-direction
 - K is the number of columns along the Z-direction
 - F is the data format. Note that only the POINT format is supported by Flex
- 4. Data block includes the coordinates and data values. Each row must contain single-space-delimited values corresponding to the variables specified in Item 2 above. Rows must be in ordered first by layer (K), then by row (J), and finally by column (I). A FORTRAN routine to write the data would look something like:

```
D0 k = 1 to nlay
D0 j = 1 to ncol
D0 i = 1 to nrow
WRITE(*,*) X(i), Y(j), Z(i,j,k), (COND(i,j,k,l), l=1,nvar)
END D0
END D0
END D0
```

An example dataset follows:

TITLE = "Simple 3D-Volume Conductivity Data"
VARIABLES = "X", "Y", "Z", "Kx", "Ky", "Kz"
ZONE I=3, J=4, K=3, F=POINT
1.0 2.0 1.1 2.21 2.21 0.221
2.0 2.1 1.2 5.05 5.05 0.505
3.0 2.2 1.1 7.16 7.16 0.716
1.0 3.0 1.2 3.66 3.66 0.366
2.1 3.2 1.5 10.1 10.1 0.101
3.1 3.4 1.3 13.8 13.8 1.380
1.0 4.0 1.3 5.21 5.21 0.521
2.2 4.4 1.4 13.4 13.4 1.340

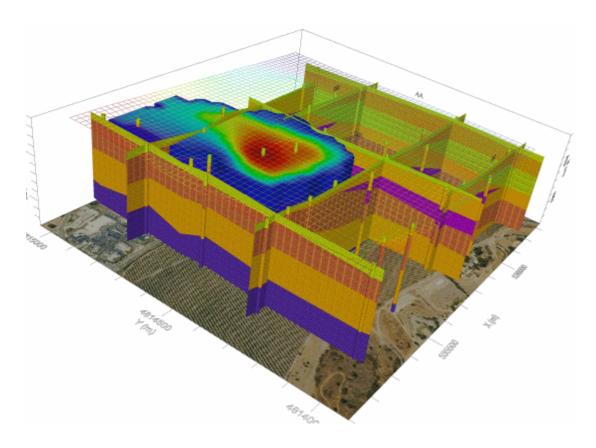


Imported example dataset, as displayed in Visual MODFLOW Flex.

4.1.7 HGA Cross-Sections

Visual MODFLOW Flex is capable of importing 3D cross-sections generated by Hydro GeoAnalyst (HGA) data management software.

For information on how to create 3D cross-section in HGA, please refer to the HGA User's Manual. For HGA product information, please visit the HGA product website: <u>www.waterloohydrogeologic.com/hydro-geoanalyst/</u> or contact your sales representative or local distributor.



When a cross section is created in HGA's 3D Explorer, a file (*.3XS) is saved in the v3D folder, located in the HGA project folder. By default, the location of this folder is:

C:\Program Files\HGAnalyst\Projects\[Project Name]\Scene\v3D

A *.3XS file contains information on the wells and layers of each cross section. The cross section can contain geology, hydrogeology, and model layer interpretation layers. When imported into VMOD Flex, this data can be used for generating surfaces and horizons from interpretation layers, or simply for visualization purposes.

To import a cross section file in VMOD Flex, follow the steps below:

- Right-click in the Data Explorer and select Import Data... from the pop-up menu.
- Select Cross Section from the Data Type drop down list.
- Click the [...] button and locate the source file.
- Enter a Name and a Description for the data, and click [Next] to continue
- Next, select the Coordinate System of the cross section. If the coordinate system is different than the one defined in the project settings, VMOD Flex will perform a geotransformation, converting all coordinates to the project's coordinate system. Click the [Next] button to continue to the next step.
- The final step involves selecting the elevation units and previewing the cross section data.

🐯 Data Import			_		\times
Define the elevation units meters	~				
Source file data					
Number of Cross sections 4	Number of Wells 14	Number of Interpretation 3			
Cross section names	Well names	Interpretation names			
AA BB CC DD	GB-01 ^ GB-02 GB-04 GB-05 GB-06 GB-12 v	Model Geology Hydrogeology			
		< <back c<="" finish="" td=""><td>ancel</td><td>Help</td><td>þ</td></back>	ancel	Help	þ

At the top of the dialog, specify the cross section elevation units from the drop-down list box. You can choose from meters or feet.

The Source File Data frame contains information about the selected source file. Here you can preview the Number of Cross sections in the source file, along with the cross section names. The Number of wells in the source data is shown, along with the well names. Finally, the number and type of interpretations in the source data are shown, e.g., Model, Geology and Hydrogeology.

Click the [Finish] button to import the cross section data. Upon importing, a new cross section data object will be added to the Data Explorer.

4.1.8 Time Schedules

Time schedule data generally contains time data for one or more attributes. It can be used in Visual MODFLOW Flex to define the stress periods for transient boundary condition attributes, e.g., recharge, river stage etc. or to define observations. The following file types are supported for time schedule data:

• Excel (*.XLS)

Time schedule data can be imported using either an absolute or relative time format. An example of an absolute time schedule is shown below:

Time	River Stage
11/01/2008	16.18
11/15/2008	16.01
12/01/2008	16.12
12/15/2008	16.29
etc	

An example of a relative time schedule is shown below:

Starting Date:	11/01/2008
Time	River Stage
0	16.18
15	16.01
30	16.12
45	16.29
etc	

To import time schedule data, follow the steps below:

- Right-click in the Data Explorer and select Import Data... from the pop-up menu.
- Select Time Schedule from the Data Type drop down list.
- Click the [...] button and locate the source file.
- Enter a Name and a Description for the imported data, and click [Next] to continue.
- The next step allows you to preview the source data before importing, and choose a subset of the source data, e.g., a worksheet of an excel file. Select which Excel worksheet to import from the Select Worksheet drop down list. Also, you can choose which row to import from using the From Row text field.
- The next step involves selecting the type of time data used in the source file.

e and Time format ir Relative	Start date		Start tir	ne		
	5/ 1/2012			MA 00	\$	
) Absolute	Date format	ate format		Time format		
	M/d/yyyy		→ h:mm t	t	~	
eview						
Date	Time	stage	recharge	EndTime	stage2	stage-tc ^
2012-05-01T00:0	1899-12-30T12:00:00-05:00	20.85	39	1	17.85	240.85
2012-05-02T00:0	1899-12-30T12:00:00-05:00	20.96	64	2	17.96	240.96
2012-05-03T00:0	1899-12-30T12:00:00-05:00	20.42	96	3	17.42	240.4200
2012-05-04T00:0	1899-12-30T12:00:00-05:00	20.62	11	4	17.62	240.62
2012-05-05T00:0	1899-12-30T12:00:00-05:00	20.44	26	5	17.44	240.44
2012-05-06T00:0	1899-12-30T12:00:00-05:00	20.18	23	6	17.18	240.18
2012-05-07T00:0	1899-12-30T12:00:00-05:00	20.99	26	7	17.99	240.99
2012-05-08T00:0	1899-12-30T12:00:00-05:00	20.84	97	8	17.84	240.84
2012-05-09T00:0	1899-12-30T12:00:00-05:00	20.99	21	9	17.99	240.99
2012-05-10T00:0	1899-12-30T12:00:00-05:00	20.95	63	10	17.95	240.95
2012 OF 11T00-0	1000 10 00710.00.00 05.00	20.75	77	111	17 75	>

- If the time values are expressed in relative time select the Relative option, and specify the starting date and time from the combo boxes. If the time values are expressed in absolute time, select the Absolute option.
- Click the [Next] button to continue.
- The next step involves data mapping and creating attributes. The required target fields will vary depending on which option was selected in the previous step, e.g., Absolute or Relative.

	Target	fields	Map to	Unit cate	gory	Unit	Multiplier	Data Type
• [DateTime	C	ate	None	None	1	1	DateTime
• 1	Time	Т	ime	None	None	1	1	DateTime
0	Create a new at	tribute s	tage	Length	m	1	1	Numeric
Create a new attribute recharge		echarge	Recharge	mm/yr	1	1	Numeric	
	×							
	Data Preview	Time	stane	recharge	EndTime	stane?	stage-ton-point	stane-end-point
urce		Time 1899-12-30T12:	stage	recharge	EndTime	stage2	stage-top-point 240.85	stage-end-point
urce 201:	Data Preview Date		20.85	-		-		
201: 201:	Data Preview Date 2-05-01T00:0	1899-12-30T12:	20.85 20.96	39	1	17.85	240.85	235.85
201: 201: 201:	Data Preview Date 2-05-01T00:0 2-05-02T00:0	1899-12-30T12: 1899-12-30T12:	20.85 0 20.96 0 20.42	39 64	1 2	17.85 17.96	240.85 240.96	235.85 235.96
201: 201: 201: 201: 201: 201:	Data Preview Date 2:05:01T00:0 2:05:02T00:0 2:05:03T00:0 2:05:04T00:0 2:05:04T00:0 2:05:05T00:0 2:05:05T00:0	1899-12-30T12: 1899-12-30T12: 1899-12-30T12: 1899-12-30T12: 1899-12-30T12:	20.85 20.96 20.42 20.62 20.44	39 64 96 11 26	1 2 3 4 5	17.85 17.96 17.42 17.62 17.44	240.85 240.96 240.420000000 240.62 240.44	235.85 235.96 235.4200000000 235.62 235.44
201: 201: 201: 201: 201: 201: 201:	Data Preview Date 2-05-01T00:0 2-05-02T00:0 2-05-03T00:0 2-05-03T00:0 2-05-04T00:0 2-05-05T00:0 2-05-06T00:0	1899-12-30T12: 1899-12-30T12: 1899-12-30T12: 1899-12-30T12: 1899-12-30T12: 1899-12-30T12: 1899-12-30T12:	0 20.85 0 20.96 0 20.42 0 20.62 0 20.44 0 20.18	39 64 96 11 26 23	1 2 3 4 5 6	17.85 17.96 17.42 17.62 17.44 17.18	240.85 240.96 240.420000000 240.62 240.44 240.18	235.85 235.96 235.4200000000 235.62 235.44 235.18
201: 201: 201: 201: 201: 201: 201: 201:	Data Preview Date 2:05:01T00:0 2:05:02T00:0 2:05:03T00:0 2:05:04T00:0 2:05:04T00:0 2:05:05T00:0 2:05:05T00:0	1899-12-30T12: 1899-12-30T12: 1899-12-30T12: 1899-12-30T12: 1899-12-30T12:	0 20.85 0 20.96 0 20.42 0 20.62 0 20.44 0 20.18 0 20.99	39 64 96 11 26	1 2 3 4 5	17.85 17.96 17.42 17.62 17.44	240.85 240.96 240.420000000 240.62 240.44	235.85 235.96 235.4200000000 235.62 235.44

- If you selected Absolute, the required target field will be Start Date and Time, and if you selected Relative, the required target field will be Relative Time. Map the time field in your source data to the required target field.
- Next, create a new attribute, and map any associated parameter, e.g., recharge, in the source data to the new attribute. If necessary, repeat for additional parameters in the time schedule.

Data mapping and creating new attributes are described in the "Data Mapping" section.

The final step in the time schedule import process is data validation. Visual MODFLOW Flex will validate the mapped data, and highlights any rows that contain invalid data, e.g., null values, wrong assigned data type, duplicate rows etc.

Please see "Data Validation" for more information on data validation.

Click the [Next] button to import the data. Once imported, a time schedule data object will be added in the Data Explorer.

4.1.9 Maps

Site maps of the model region, such as aerial photographs, topographic maps and satellite imagery, are often useful for gaining a perspective of the dimensions of the model, and for locating important characteristics of the model. Although maps do not contain any specific data used in the calculations, and the presence of a map does not influence the results of the simulation, they are useful for enhancing visualization of the model.

Visual MODFLOW Flex supports the following raster graphics file types:

- Bitmap (*.BMP)
- Tagged Image Format (*.TIF)
- JPEG Interchange Format (*.JPG)

Please Note: When a raster image is imported into Visual MODFLOW Flex, the source file is copied and saved in the project's data repository folder. As such, the original file may be modified, moved or deleted without affecting the imported raster image.

To import a map into Visual MODFLOW Flex, follow the steps below:

- Right-click in the Data Explorer and select Import Data... from the pop-up menu.
- Select Map from the Data Type drop down list.
- Click the [...] button and locate the source file.
- Enter a Name and a Description for the data, and click [Next] to continue
- Next, select the Coordinate System of the image file. If the coordinate system is different than the one defined in the project settings, Visual MODFLOW Flex will perform a geotransformation, converting all coordinates to the project's coordinate system.
- Click the [Next] button to continue to the next step.

All raster images must be georeferenced before importing into Visual MODFLOW Flex. If the selected raster image has already been georeferenced, it will have an associated "world" file, and as such, it will not need to be georeferenced in Visual MODFLOW Flex.

Please Note: the world file must have the same filename as the image, and must be located in the same folder as the selected source file, in order for Visual MODFLOW Flex to recognize it.

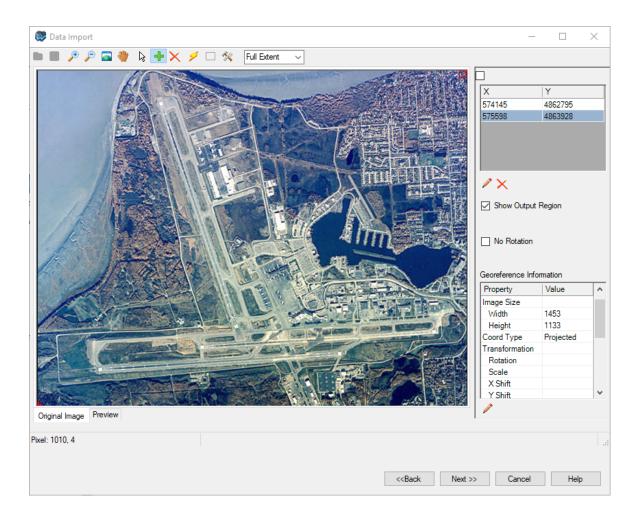
The following table summarizes the supported graphics file types, and the corresponding georeferencing tag files:

Raster Source	Corresponding World File
*.BMP	*.BPW
*.TIF	*.TFW
*.JPG	*.JPW

If your source image has a world file, you can skip to the final step. If the source file does not have a world file, you will be prompted to manually georeference the raster image. This procedure is described in the following section.

Georeferencing Images

Georeferencing a graphics file involves mapping a coordinate system to the individual pixels of the image. When this is required, the following window will display, when importing a raster image:



Toolbar Buttons

The buttons in the top toolbar are described below:

- Zoom In: Click-and-drag the mouse to select the zoom area.
- Zoom Out: Zoom out of the image.
- Full Extent: Zoom completely out so that the entire image is shown.
- Pan: When zoomed in, move the image left, right, up or down.
- Add (Control Point): Add a georeference point. See "Adding Georeference Points".
- Delete (Control Point): Delete a selected georeference point.

 Transform Image: Assigns coordinates to image pixels using the specified control points.

Output Region: This button allows you to save a specified area of the image to the georeferenced file, after the image has been transformed. By default, the output region is the whole image. Click-and-drag a rectangular box on the image to define a new output region, and then click the Save button to save the output region to the georeference file.

Configure Georeferencing Options: Opens the configure georeferencing options dialog box. For more information on these options, please see "Configure Georeferencing Options" section.

Magnification Selector: Select a magnification level from the combo box.

Control Points Table

The control points table contains the specified control points. You can edit an existing control point by selecting the point from the table, and then clicking the Edit button. A dialog box will display prompting you to modify the control point coordinates.

You can also delete a control point from the control points table. To do so, select an existing control point from the grid, and then click the Delete button.

Georeference Information Table

The georeference information table displays information about the georeferenced image including the original image file name and path, the original image size, and coordinate type (projected, local or geographic). It also displays information on the transformation such as the degree of rotation, scale X-Y shift, and the output file name path and image size.

Georeference Info	ormation
Property	Value
Image File	Q:\VM5\6-Testin
Image Size	
Width	1453
Height	1133
Coord Type	Projected
Transformation	
Rotation	-0.07
Scale	1.006
X Shift	574,140.98
Y Shift	4,862,789.96
Output File	Q:\VM5\6-Testin
Output Region	
Left	574,196.01
Тор	4,863,897.78
Width	127.27
Height	74.07
Output Size	
Width	127
Height	75
1	

Adding Georeference Points

In order to map pixels of the image to a coordinate system, the image must have at least two georeference points with known world coordinates. To set a georeference point:

- From the top toolbar, click on the Add button.
- Click on a map location where the world coordinates are known.
- A georeference point window will appear prompting for the X and Y world coordinates of the selected location.
- Enter the X and Y coordinates for this point.
- Repeat this procedure for additional georeference points.
- When you set a georeference point, it is added to the Control Points Table.

You can improve the accuracy of the georeferencing by adding more than two control points to the image. When the image is transformed, the Preview tab will display the original control points and the corresponding georeferenced points, thus allowing you to visualize the accuracy of the georeferencing.

Once you have set at least two georeference points, click the Transform button to georeference the image. The georeferenced image will then be displayed in the Preview tab.

Editing Georeference Points

To edit a georeference point:

- Select the georeference point from the Control Points Table
- Once selected, click the Edit button (located just beneath the control points table)
- A Georeference point window will appear prompting for the X and Y world coordinates of the selected location.
- Enter the new X and/or Y coordinates for this point.
- Click the [OK] button.

Please Note: You must click the Transform button again in order for the georeferencing to update to reflect the modified X-Y values.

Deleting Georeference Points

To delete a georeference point:

- Select the georeference point from the Control Points Table.
- Once selected, click the Delete button (located just beneath the control points table)

Configure Georeferencing Options

When the Configure Georeferencing Options button is selected, the following dialog will open:

Settin	ngs						\times
Syr	mbols	Geor	reference Image				
	Orgin	al Poi	nts		Georefere	nce Points	
	Styl	е	CrossCircle	\sim	Style	Circle ~	
	Size	e	12	-	Size	8	
	Cole	or			Color		
				_			
			\				
	1				J		
			Apply	ОК	(Cancel	

Symbols Tab

This tab allows you to change the style settings of the original control points and the georeference points. Choose a Style, symbol Size and Color. A preview of the symbol settings is shown in the boxes below.

Georeference Image Tab

This tab allows you to define settings for the georeferenced image. Each setting is described below.

S	Settings	\times
	Symbols Georeference Image	
	Show Fill Color	
	Fill color for empty area	
	JPEG image quality L	
	Interpolation Mode Default ~	
	Apply OK Cancel	

When a georeferenced image is rotated, you can fill the areas of empty space with a specified color. Otherwise, leave the check box unchecked and the empty space will show transparent.

Click the color box beside Fill color for empty area to select the color to fill the empty spaces (only if Show Fill Color option is selected).

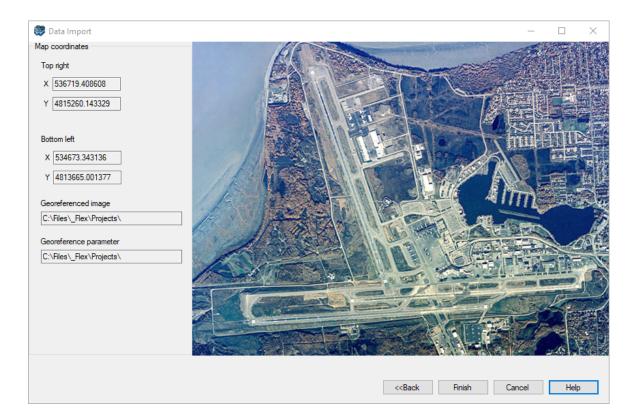
Use the slider to set the JPEG Image Quality. When set closer to L (low), more compression is used in the saved georeference image file, resulting in a smaller file and poorer quality. When set close to H (high), less compression is used in the saved georeferenced image file, resulting in a larger file with better quality.

From the Interpolation Mode combo box, specify the interpolation method (algorithm) to use when the image is scaled or rotated The various interpolation methods are briefly described below. Keep in mind, lower-quality interpolation mode will result in a smaller output file, whereas high-quality interpolation modes will result in a larger output file.

- **Bicubic**: Bicubic interpolation. No prefiltering is done. This mode is not suitable for shrinking an image below 25 percent of its original size.
- **Bilinear**: Bilinear interpolation. No prefiltering is done. This mode is not suitable for shrinking an image below 50 percent of its original size.
- Default: Default interpolation mode
- **High**: a high-quality mode.
- **HighQualityBicubic**: High-quality, bicubic interpolation. Prefiltering is performed to ensure high-quality shrinking. This mode produces the highest quality transformed images.

- **HighQualityBilinear**: Specifies high-quality, bilinear interpolation. Prefiltering is performed to ensure high-quality shrinking.
- Invalid:
- Low: a low-quality mode.
- NearestNeighbor: Nearest-neighbor interpolation.

The final step involves previewing the raster image and viewing coordinate information, before importing into Visual MODFLOW Flex.



The Map Coordinates frame provides the georeferenced coordinates of the Top Right and Bottom Left corners of the image. The path of the georeferenced image, and the associated georeference tag file is also shown.

Click the [Finish] button to import the map into Visual MODFLOW Flex.

4.1.10 DXFs

Site plans and other spatial information can be useful for gaining a perspective of the dimensions of the model, and for locating important spatial features within the model domain. Although these maps may not contain any specific data used in the calculations, and the presence of a map does not influence the results of the simulation, they are useful for enhancing visualization of the model and in the decision making-process (e.g. what are the simulated results within a given property line?).

Visual MODFLOW Flex supports import and visualization of AutoCAD drawing exchange files (DXFs) for use as a vector basemap.

Import a DXF file

To import a DXF into VMOD Flex, follow the steps below:

- Right-click in the Data Explorer and select Import Data... from the pop-up menu.
- Select DXF from the Data Type drop down list.
- Click the [...] button and locate the source file.
- Enter a Name and a Description for the data, and click [Next] to continue
- Next, select the Coordinate System of the image file.
- Click the [Next] button to continue to the next step.
- A summary of the number of DXF entities processed and the number that will be created in Flex will be displayed
- Click the [Finish] button to finalize the import.

You can import points, polylines, or polygons that exist within a DXF file separately.

Limitations

The following limitations apply to importing DXF files:

- The coordinate system of the DXF file must be consistent with the one defined in the project settings as Flex will not perform a geotransformation on entities within the DXF.
- When importing Points, Polygons, or Polylines from a .DXF file, only the entities within the .DXF \$EXTMIN and \$EXTMAX will be imported; any entities outside these extents will not be imported. Therefore, please be sure to prepare your .DXF file properly, prior to importing.
- All entities within the DXF file will be processed for import and any compatible entities will be imported into the project and displayed using the same color. Some entities are not supported and may cause errors on import. As such, it may be useful to remove entities that are not relevant to the model prior to import.

 Point, polyline, and/or polygon entities imported into Visual MODFLOW Flex as part of a DXF import cannot be used to develop conceptual model elements, such as model extents or boundary conditions. You must import these entities separately as <u>points</u>, <u>polylines</u>, or <u>polygons</u>.

4.1.11 Validation

Data Validation

The final data import step involves validation of the data being imported. This step will ensure that the records in the imported data set contains valid data for each of the mapped fields.

<mark>ല</mark> Data Import								_			
There are 1 records with errors, highlighted in red. These records will not be imported. Source 'Kx (ft/day)' contains ilegal numeric value "											
Do not import rows with warnings Mapped Data Preview 20 records were mapped Show only errors and warnings Show this amount 100											
Apply											
Row	X	Y	Elevation	Kx (ft/day)	lay2	lay3	Errors	lay4			
J 1	575150	4863000	16.5	-9999	10	8.1	Error	0.1			
					< Back	<u> </u>	Cancel	telp			

In the top half of the dialog, Visual MODFLOW Flex will list any mapped fields that contain invalid data, along with a reason for why they are deemed invalid. The data validation rules for each mapped column are as follows:

- X and Y values must be a numeric value, and present in each row of the mapped data.
- Data columns will be deemed invalid if Visual MODFLOW Flex detects a null (blank) field.
- Data in each column must satisfy the specified data type (e.g. a column denoted as numeric will return errors for rows containing a string in that column).

If invalid data exists, you can choose to import this data anyway. Otherwise, you can select the Do Not Import Rows with Warnings check box, and Visual MODFLOW Flex will not import any rows deemed invalid.

In the bottom half of the dialog, there are two options:

- Show only errors and warnings: When selected, only the records deemed invalid will be shown in the preview table. Records that are deemed invalid will be colored either red (error) or yellow (warning).
- Show this amount: When selected, you can view a specified number of records in the preview table below. Enter a value, and then click the [Apply] button to show the records (both valid & invalid) in the preview table.

When you import pumping well schedule data or head/concentration observation data in Absolute time format, Visual MODFLOW Flex will check the date values against the start date you defined in the modeling objectives;

- For pumping well schedules, any wells that have dates before the model start date will be flagged as warning, since these data cannot be used when you create Pumping Wells Boundary condition object. Likewise
- For head/concentration observations, any wells that have dates before the model start date will be flagged as warnings, since these observations cannot be used as calibration points in the numerical model.

Click the [Finish] button to import the data. Once imported, a data object will be added in the Data Explorer.

4.2 Importing VMOD/MODFLOW Models

Importing Visual MODFLOW Classic Projects

To import your Visual MODFLOW Classic project, select the .VMF file and click OK to continue. The .VMF file must be from Visual MODFLOW v.2009.1 or later.

If your Visual MODFLOW Classic project contains Transport Boundary condition parameters, please refer to the <u>discussion</u> on the differences between how Classic and Flex handle point source concentrations for more details.

While the model is created, you will see the corresponding inputs added to the Model Explorer.

Importing MODFLOW Data Sets

Often you may need to import an existing MODFLOW data set into Visual MODFLOW Flex in order to review the model, or evaluate different scenarios. Visual MODFLOW Flex can import existing MODFLOW data sets provided they are in MODFLOW-2000, MODFLOW-2005, or MODLFOW-NWT format. Visual MODFLOW Flex does not currently support direct import of MODFLOW-SURFACT or SEAWAT data sets. These must be imported as part of a Visual MODFLOW Classic project file. Import of MODFLOW-USG or MODFLOW-6 projects is also not yet supported in Visual MODFLOW Flex.

Limitations

Visual MODFLOW Flex allows you to import finite difference models with the following limitations:

Engines

Visual MODFLOW Flex currently imports MODFLOW-2000, -2005, and -NWT Groundwater Flow process files only. As a result, it will ignore files associated with the Sensitivity Process, the Observation Process, the Parameter Estimation Process, and the Transport Process.

Packages

The following packages are not supported for import and must be commented out (by adding a # character to the first column where each unsupported package is invoked) in the MODFLOW name (.NAM) file prior to import:

 CFP, DRT, LVDA, MNW1, MNW2, MNWI, MULT, RES, SFR, STR, SUB, SWI2, SWT, UZF, ZONE

Packages that include so-called PARAMETER inputs, as described on p8-2 to 8-7 in the MODFLOW-2005 manual (Harbaugh, <u>2005</u>), may also cause failures with the import process.

Although not supported directly for import, many of these packages can be rebuilt in Flex (MNW1, MNW2, MNWI, SFR) or added indirectly to the model run using the <u>Advanced</u> <u>Settings</u> at the translation step.

Importing the model

To import a MODFLOW-2000, MODFLOW-2005, or MODFLOW-NWT model data set, select the .NAM file (or .MODFLOW.IN) at the Import Grid step.

Please Note: The .NAM file (or .MODFLOW.IN file) is an ASCII file containing a list of the input and output data files for the model, and their location (folder and pathname) on the computer. If the model files have been moved to a new location, the file must be manually updated to reflect the new file location(s).

Once you have selected the desired model data file, click on the [Open] button to continue.

Working w	vith Your	Data	353

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4.2.1 Transport



Visual MODFLOW Flex to Visual MODFLOW Classic: Transport Boundary Conditions



If you are used to working with Visual MODFLOW Classic, you will notice a difference in how transport boundary conditions are handled in Visual MODFLOW Flex. In Visual MODFLOW Classic, transport boundary conditions were defined separately from the flow boundary conditions using the types Constant Concentration, Recharge Concentration, Evapotranspiration Concentration, and Point Source. In Visual MODFLOW Flex, the sink/source parameters for transport models (which are time and species concentrations) are defined as part of flow boundary conditions, which is a more natural representation. This means you do not define separate cell geometries for transport boundaries, you simply define species concentrations while defining the flow boundary conditions, where required. Constant Concentration is an exception to this rule, since it does not need to coincide with a prescribed flux, you will still see a "Constant Concentration" boundary condition type, allowing you to define the geometry (cells) and parameters (time and species concentrations) for this Boundary Condition type.

When Transport is active in your model run, and you define a new boundary condition, you will see parameters for Species Concentration as part of the Boundary Condition attributes (eg. Conc001, Conc002, etc.). These will have a default value of -1, indicating that no mass sink/source is defined for this group of boundary condition cells. As soon as you change this value to 0 or greater, then these cells will be treated as sinks/sources.

Time Schedule:

Currently in Visual MODFLOW Flex when you import a Visual MODFLOW Classic model with point source concentrations, the program assumes that the time schedule for the point sources are the same as that of the flow boundary condition to which it is assigned; if it is necessary to have a different time schedule, then please re-define the flow boundary condition with the necessary time adjustments, then re-assign the point source concentrations.

Point Source assigned to Cells instead of Well Screens:

In Visual MODFLOW Classic point source concentrations were assigned to cells, and not to the screened interval. In this fashion, it is possible to have different point source concentrations over the screened interval (over different model layers). This configuration is not supported in Visual MODFLOW Flex. When you import a Visual MODFLOW Classic model and this scenario is encountered, you will receive a warning message about affected wells. Please verify and fix these wells before proceeding.

Multiple Wells in the Same Cell:

In Visual MODFLOW Classic, multiple wells could belong to a cell, however point source concentrations were assigned to a cell. In Visual MODFLOW Flex, point source concentrations are assigned directly to the well screen, which is a more natural approach. If you import a model from Visual MODFLOW Classic, and it detects that there are multiple wells in a cell that also contains a point source concentration, you will receive a warning during import with a list of the affected wells. Please verify and fix these wells before proceeding.

4.3 Creating Surfaces

In Visual MODFLOW Flex, a surface refers to an attribute (e.g., elevation, conductivity, heads) represented as a set of continuous data over an area. Surfaces can either be imported directly (see <u>"Importing Surfaces</u>") from various file types using the import utility, or created by interpolating one or more points data objects. This chapter describes the process of creating surfaces from point data objects.

Surfaces are required in Visual MODFLOW Flex for defining the vertical boundaries of structural zones, e.g., horizons in a conceptual model. However, surfaces can also be used to assign spatially-variable attributes to property zones and boundary conditions, or for simply visualizing spatial variation using the 2D or 3D Viewers.

The create surface process allows you to generate surfaces using any numeric attribute in a point data object. The point data object can be one that has been imported using the import utility, or one that has been generated from other data objects, e.g., cross sections and wells.

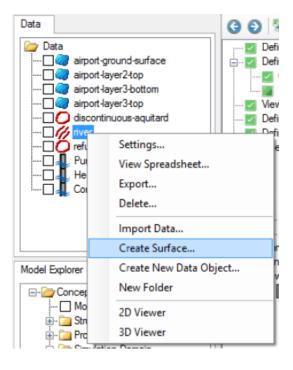
This chapter presents information on the following topics:

- <u>Create Surface</u>
- General Settings
- Interpolation Settings

Create Surface

To create a new surface, follow the steps below:

• From the Data Explorer, right-click anywhere and select Create Surface... from the pop-up menu.



• The Create Surface dialog will display. Specify the general settings, described in the following section.

*	Creat	e Surface		×
General Settings	Interpolation Settings			
Surface Name:*				
Surface1				
Description				
Data Source*				
Data Object		Z Value		
				$+$ \times
		<u>O</u> K	<u>C</u> ancel	<u>H</u> elp

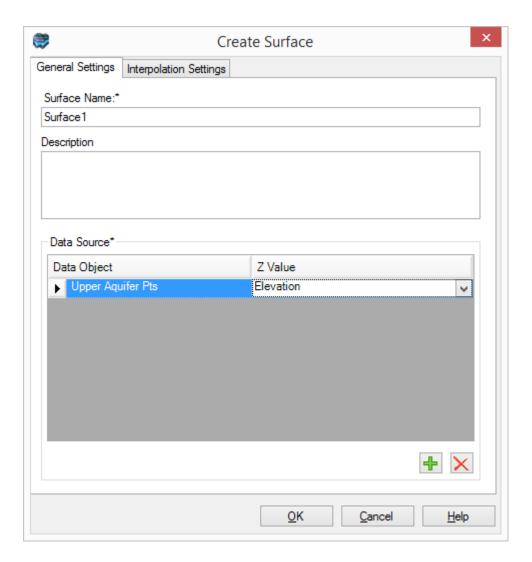
General Settings

Enter a unique name for the surface in the Surface Name field, and a description of the surface (optional) in the Description text box.

The Data Source frame allows you to select the point data object(s) from which the surface will be created.

Adding a Data Source

- From the Data Explorer, select the desired Point data object from which the surface will be interpolated.
- Click the 🖶 Add button, to add the point data object to the Data Source frame.
- Visual MODFLOW Flex allows you to create a single surface from multiple point data objects. Repeat the steps above to add additional points data objects to the Data Source frame.
- For each data source, select the Z Value from the combo box (shown below). The Z value can be any numeric attribute stored in the points data source, e.g., Elevation, Conductivity, Initial Concentration, etc.



Next, click the Interpolation Settings tab to define the interpolation settings for the surface. These settings are described in the following section.

Interpolation Settings

Select the interpolation method to use for generating the surface. Choose from the following interpolation methods:

- Inverse Distance
- Kriging
- Natural Neighbor

Gen	eral Settings	Interpolation Settings		
	Interpolation	Method	Inverse Distance	~
⊿	General			
	Min Valu	ue *	1598.31	
	Max Val	ue *	1648.67	
	Interpola	ate Log Values	No	
⊿	Grid Settings			
	Xinterva		50	
	Yinterva		50	
⊿	Interpolation			
	X Max *		2117289.4	
	Y Max *	,	606831.47	
	X Min *		2084544.72	
	Y Min *		578278.26	
⊿	Advanced S	-		
	Number	of Neighbors	10	
The	terpolation D	method is used to interpo	plating	
	⇒	3		

Below are brief descriptions of each interpolation method, taken from the GSLIB Geostatistical Software Library and User's Guide (<u>Deutsch and Journel, 1998</u>). For a description of each interpolation parameter setting, click on the setting, and a brief description will be displayed beneath the interpolation settings grid.

Once the settings have been defined, click the [OK] button to generate the surface.

Inverse Distance

The Inverse Distance Squared method is very fast and efficient, weighted average interpolation method. The weighting factor applied to the data depends on the distance of the point from the grid cell, and is inversely proportional to the distance squared. Consequently, the greater the distance the data point is from the grid node, the smaller the influence it has on the calculated value.

The Inverse Distance Squared method for interpolation may generate patterns similar to the "bull's-eye" surrounding points of observations. Selecting a larger number of nearest neighboring data points may smooth this effect, but if the bull's eye pattern is undesirable, then other methods for interpolation, like Natural Neighbor and Kriging, are recommended.

Kriging

Kriging is a geostatistical method that produces visually appealing maps from irregularly spaced data. Anisotropy and underlying trends suggested in raw data can be incorporated in an efficient manner through Kriging. The program used, called kt3d, is available in the public domain from the Geostatistical Software Library (GSLIB), distributed by Stanford University, and is well documented by Deutsch and Journel (1998). The project kt3d performs simple Kriging, ordinary Kriging, or Kriging with a polynomial trend, and uses the standard parameter file used by GSLIP. If the semi-variogram components have already been modeled by the user, they can be incorporated into the program by choosing the appropriate set of parameters in the parameter file. The semi-variograms available include Spherical, Exponential, Gaussian, Power, and the Hoe effect models. If the variogram information is not available, the default linear variogram with no nugget effect should be used. This option is a special case of the Power model with the exponent equal to 1. When using the Kriging interpolation method, you may need to adjust the min and max radii of the variogram in order to get an ideal interpolation; these parameter values will depend on your data set. Default values are 100 and 100 along the major and semi-major axes. You will likely need to alter these values based on your input dataset and on the characteristics of the model domain.

Natural Neighbors

The Natural Neighbor method (Watson, 1994) is based on the Thiessen polygon method used for interpolating rainfall data. The grid node for interpolation is considered a new point, or target, to the existing data set. With the addition of this point, the Thiessen polygons based on the existing points are modified to include the new point. The polygons reduce in area to include the new points, and the area that is taken out from the existing polygons is called the "borrowed area". The interpolation algorithm calculates the interpolated value as the weighted average of the neighboring observations where the weights are proportional to the borrowed areas. The Natural Neighbor method is valid only with the convex hull of the Thiessen polygon formed by the data points, and values outside the hull extrapolation should be used with caution.

The Natural Neighbor interpolation scheme may be visualized as a taut rubber sheet stretched to satisfy all the data points. The interpolated value at any location is a linear combination of all Natural Neighbors of that location, and the resulting surface is continuous with a slope that is also continuous. Combining the gradients or slopes with the linear interpolation provides results that are more smooth, and may anticipate the peak and valleys between data. Singularities and other undesirable effects may be lessened by incorporating the gradient factor.

The gradient influence on the results can be manipulated by two tautness parameters that you can enter. These parameters allow the interpolated surface to vary from purely linear interpolation to one which is well rounded and has a gradient factor. In all cases the slope discontinuities are removed and the resulting surface has slope continuity everywhere.



Interpolation Settings

Data object spreadsheet tables can be viewed by rightclicking on the data object in the Data Explorer, and selecting Spreadsheet... from the pop-up menu. 2D Viewers can be set to pick mode by selecting the Pick Mode button from the viewer sidebar.

Defining an Interpolation Domain using a Polygon

When creating a surface, the interpolation domain is automatically calculated from the X and Y extents of the specified point(s) data set. There may be times when you do not want to use the entire points data set to generate a surface. In this case, you can manually define the interpolation domain (Xmax, Ymax, Xmin, Ymin) by specifying new values in the interpolation settings grid, or you can use an imported or digitized polygon data object.

- To define the interpolation domain using a polygon data object, follow the steps below:
- In the Create Surface dialog box, select the Use a polygon extent check box.
- Select a polygon data object from the Data Explorer, and then click the 📄 button.

Interpolation Domain					
× Max *	574438.89028680592				
Y Max *	4863746.207869472				
X Min *	573851.95385850687				
Y Min *	4863459.610148631				
Advanced Settings					
Number of Neighbors	10				
Interpolation Domain					
Use a polygon extent					
Polygon_boundary					
	<u>O</u> K <u>C</u> ancel <u>H</u> elp				

• When the polygon data object is selected, the interpolation domain values in the settings grid will update with the X-Y extents of the selected polygon data object.

4.4 Creating New Data Objects

The 2D Viewer provides interactive drawing tools which allow you to create your own polygon, polyline and point data objects. This feature can be useful for digitizing boundary condition areas, property zones or your conceptual model boundary. To create a new polygon, polyline or points data object, follow the steps below.

• In the Data Explorer, right-click and select Create New Data Object from the pop-up menu. The following dialog will display:

	Create New Data Object ×
E E	Data Type *
	Point v
	Data Name * Point3 Load
	LUad
[<u>O</u> K <u>C</u> ancel <u>H</u> elp

- Select the Data Type from the combo box. You have the following options:
 Point
 - Polyline

 - Polygon
 - Well Set (geometry defined using tabular inputs see the section on <u>Defining</u> <u>Pumping Wells</u> in the Conceptual Model workflow)
- Enter a name for the Data Name field
- Click the [OK] button to create the new data object

Once created, the new data object will appear in the Data Explorer. From here, you can define the geometry of the data object using the 2D Viewer editing tools.

Digitizing & Editing Geometry in 2D Viewers

The 2D Viewer allows you to create and modify the geometry of points, polylines and polygon data objects. The geometry of well set data objects cannot be modified using a 2D Viewer, however, it can be modified using its <u>data table</u>. The process of drawing in a 2D Viewer is described below:

- Open a 2D Viewer by selecting Window from the Visual MODFLOW Flex main menu, and then clicking New 2D Window.
- Next, display the data object that will be edited in the 2D Viewer. **Note:** You can have multiple data objects displayed in the viewer while you're editing/drawing the data

object. However, make sure that the data object being edited is the "active" one by selecting the data object name from the Layer combo box, located at the bottom of the 2D Viewer window.

- From the 2D Viewer sidebar, select the Rick button to set the 2D Viewer to pick mode. Pick mode allows you to click and select individual shape elements, e.g., vertices, line segments, features, that comprise the active data object.
- From the 2D Viewer sidebar, select the Add button to set the 2D Viewer to edit mode. Once this button is selected, a set of editing buttons will display in the 2D Viewer sidebar. The edit buttons that show in the sidebar will vary depending on which type of data object is being edited. For example, the Add Points button will not be shown when you are editing/creating a polygon or polyline data object. The edit buttons are described below.
 - Add Points: Digitize points in the 2D Viewer by moving the mouse cursor to the desired location and clicking the left mouse button. This button only shows when creating/edit a Points data object.
 - Add Polyline: Digitize a polyline in the 2D Viewer. Click the leftmouse to start the line, and then left-click to insert a vertex along the line path. Double-click to end the polyline. This button only shows when creating/editing a Polyline data object.
 - **Add Polygon**: Digitize a polygon in the 2D Viewer. Click the leftmouse button to start the polygon. Each successive left mouse-click will insert a vertex. Double-click to close the polygon..
 - Move Points: Move a point by selecting and dragging the points to a new location in the 2D Viewer.
 - **Rescale**: Select a shape element and stretch or shrink the geometry by selecting and dragging a side or corner of the blue box.
 - Content of the second secon
 - **Delete Shape**: Delete the selected shape.
 - Undo All: Undo all edits. This button will revert the data object back to its original geometry.

If you are editing an existing polyline or polygon data object, the Selector combo box located at the bottom of the 2D Viewer allows you to select and modify the points (vertices) that comprise the features in the data object. For example, if you are editing a polyline data object, you can select Points from the Selector combo box, and each vertex that comprises each polyline will become active, allowing you to add, move or delete the vertices. When the Selector combo box is set to Points, the following icons are added to the 2D Viewer sidebar.

Add Vertex: Add a vertex to a polyline or polygon feature by placing your mouse in the desired location on the line or polygon boundary, and clicking the left mouse button.

- **Move Vertex**: Select and hold the left mouse button and move the vertex to a new location the line or polygon boundary.
- **Delete Vertex**: When selected, select a vertex to remove from a line and or polygon boundary.

Once you have created/modified the data object geometry using the edit tools described above, click the 📓 End Edit button to save the changes.

Finally, click the 🔯 View button to return to the normal 2D Viewing mode.

4.5 Deleting Data Objects

To delete a data object, right-click on the data object from the Data Explorer, and select Delete from the pop-up menu.

5 Visualizing Data in 2D/3D

Visual MODFLOW Flex supports two types of interactive data viewers: 3D Viewer and 2D Viewer. The 3D Viewer is based on OpenGL graphics technology, allowing you to visualize graphically-rich three-dimensional representations of your data. The 2D Viewer allows you to view your data from a plan perspective, and provides various tools for editing and drawing data objects.

Visual MODFLOW Flex allows you to have multiple viewers opened and displayed simultaneously. Both viewers can be launched by clicking on Window from the main menu, and then selecting New 2D Window or New 3D Window.

This chapter presents information on the following topics:

- <u>Creating Viewers, Opening, and Adding Data Objects</u>
- Working With Viewers
- <u>Viewer Controls</u>
- <u>Adjusting Viewer Settings</u>
- <u>3D Viewer Animations</u>
- Exporting Views

See Also:

- Style Settings for details on customizing how individual data layers are displayed
- Export for details on exporting data from a viewer
- Exporting 2D/3D Views to image

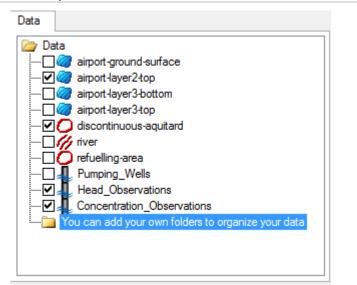
5.1 Creating Viewers, Opening, and Adding Data Objects

Opening a new 2D or 3D Viewer

There are two ways in which you can launch a 2D or 3D Viewer in Visual MODFLOW Flex: From the Main Menu or from the Data Explorer.

- From the main menu, select Window, then either 2D or 3D Viewer
- From the Data or Model Explorer, right-click on a data object and select 2D Viewer or 3D Viewer from the pop-up menu. A new viewer will then launch, displaying the selected data object. Please note that the viewers listed in the pop-up menu depend on which data object is selected (see table under "<u>Displaying Data in Viewers</u>").

Adding Data Objects to the Viewer



data in a viewer, select the check box beside the data object in the Data Explorer or Conceptual Model Explorer. If multiple viewers are opened, the data will be shown in the active viewer (denoted by a blue title bar). To remove data from a viewer, select the check box beside the data object so that it appears empty or "unchecked

To display

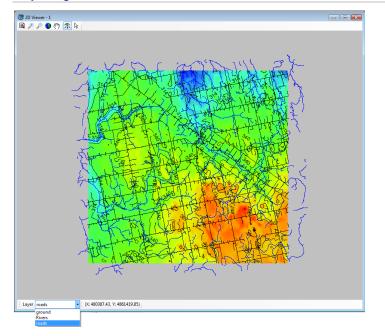
Pleas e Note: some data objec

".

ts may not be

viewa ble in the 3D or 2D View ers. (e.g. grid objec ts cann ot be viewe d in a 2D viewe r) When a data object is displayed in a viewer, it will appear as defined in the data object settings. For more information on viewing and modifying data object settings, please see Data Settings.

Layering Order in 2D Viewer



Layer ordering in 2D Viewer is determined by the sequence in which data objects are added to the viewer. For example, if data objects overlap each other, the data object added most recently will appear on top and effectively hide the underlying older data object(s).

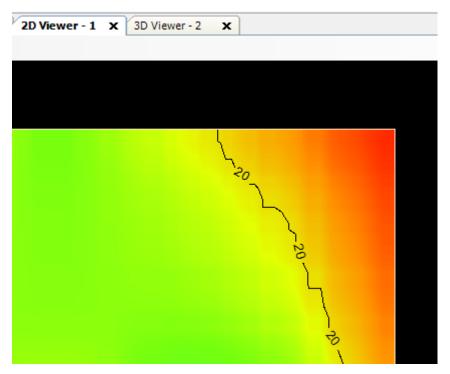
You can bring layers to the top, by using the Layer combo box, located at the top of the 2D Viewer window.

The Layer combo box contains all of the layers currently displayed in the 2D Viewer. Select a layer from the combo box to bring it to "the top" of the layer order.

5.2 Working With Viewers

Using Multiple Viewers

Visual MODFLOW Flex allows you to have multiple 2D and 3D Viewer windows opened and displayed at one time. When a new viewer is opened, it is added to the window bar, located at the top of the main Visual MODFLOW Flex Window.



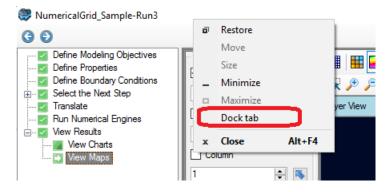
You can change the current active viewer by clicking on a different tab from the bar.

Docking/Undocking Viewers

Tabs can be undocked from the main window by drag-and-drop or by right-clicking on a tab and selecting "Undock Tab":

Sa	mple-Run4 X NumericalG	rid 🔒	Undock Tab)
	Views Views Layer 1		<u>Close</u> New Hori <u>z</u> ontal Tab Group New <u>V</u> ertical Tab Group	
	□ Row 1 ♥	Layer	/iew	

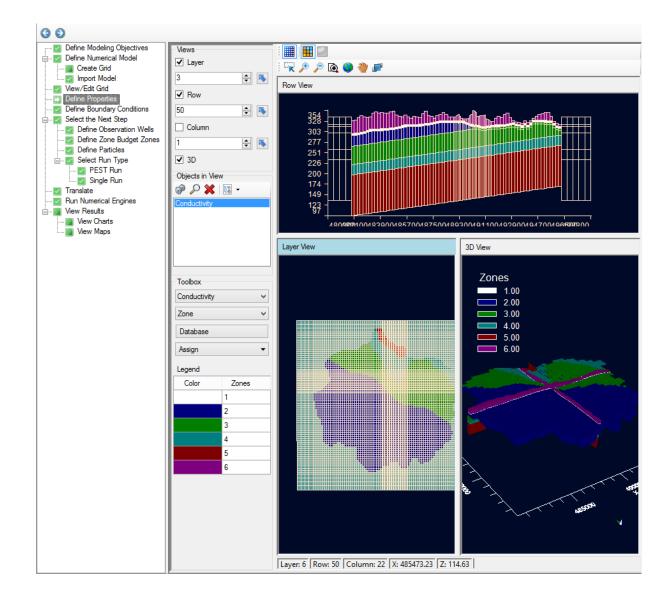
An undocked tab is displayed as a separate window that can be resized, minimized, or maximized using standard Windows controls. Multiple tabs can be undocked at the same time on multiple monitors, but at least one tab must remain docked in the main window. An undocked tab can be docked back into the main Visual MODFLOW Flex window by dragging it back on to the main window or right clicking on the window and selecting "Dock Tab":



Flex Viewer

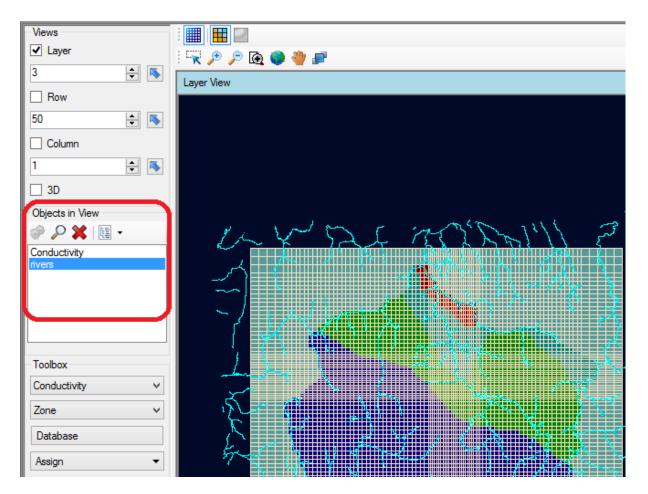
The Flex viewer is available in numerical modeling workflows for regular (MODFLOW Finite Difference) grids. This multi-purpose view gives you the ability to view and inspect your numerical model data along a selected layer, row, column, and/or 3D view.

- Under **Views**, select the various views you want to see in the Flex viewer; Visual MODFLOW Flex allows you to simultaneously show a layer, row, column and 3D Views. Place a check box beside the desired view and it will appear on the screen.
- Adjust a specific layer, row, or column using the up/down arrows. Alternatively, click on the button then click on any specific row, column, or layer in any of the 2D views, and the selected row, column, or layer will be set automatically.
- To rearrange the views, you can select the swap horizontal () and vertical () buttons in the viewer toolbar
- By default, the 3D Viewer will show a "<u>ThreeSlice</u>" view of the selected Layer, Row, and Column. For details on controlling the display of this, see <u>3D Gridded Data</u> <u>Settings</u>.



Objects in View

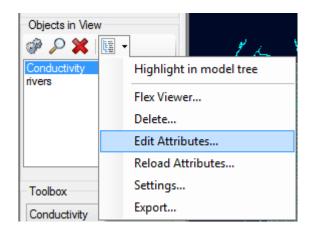
Below the list of Views you will see the Objects in View Panel.



This panel provides a list of the data objects that are visible in the current view; any objects that have been "checked on" from the Data tab or Model Explorer will be listed in this Objects in View; since both the Data tab and Model Explorer can grow in size and complexity as your project evolves, this Objects in View panel provides a nice short-cut to hide objects you don't wish to see in the view. In addition, you can access context menu options from this panel; these are menu items that were typically only available by right-clicking on the Data tab or Model Explorer.

Toolbar options (from left to right):

- Settings: loads the Settings options for that data object
- *P* **Isolate**: temporarily selects that data object in the view and hides all others; you need to click and hold down this menu option in order to maintain the selection
- X Delete (remove): removes this object from the view, but does not delete the underlying data from the project
- More Actions: Loads a context menu options similar to what you would get if you were to right-click on the object from the Model Explorer (or Data Tab); an example is shown below for "Conductivity"



Saving Views

On closing a newly created standalone (2D, 3D, or Flex) view, closing the project, or exiting Flex, you will prompted to save the new view(s) for later use. Saved views can be reloaded and managed by selecting **View > Open...** from the main menu.

5.3 Viewer Controls

The viewer controls allow you to interact with displayed data objects. The controls are accessible from the toolbar located along the top of the viewer window.

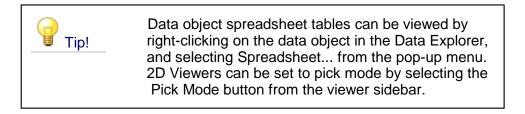
- **View Mode**: The default mode. Allows you to zoom, rotate and pan the displayed data objects.
- Pick Mode: (2D Viewer Only) Allows you to select individual data object elements currently displayed in the viewer. When in Pick Mode, the Edit button will be shown in the sidebar, allowing you to edit the selected data object element.
- Rotate: Allows you to rotate the displayed data objects using your mouse. Click-and-hold on the displayed data, and move the mouse in a direction to rotate the data. (Available in 3D Viewer only).
- Move/Pan: Allows you to move/pan the displayed data objects in the viewer.
- Zoom In: Allows you to zoom in on the displayed data objects.
- Zoom Out: Allows you to zoom out of the displayed data objects.
- **Zoom Into box**: Use the mouse cursor to draw a box around an area of interest, and automatically zoom into this area.
- Reorder layers: Allows you to move layers up/down in a 2D view. Note that the topmost layer is the active layer; when doing editing of shapes, you must first set the desired layer to be the topmost.

Cell Inspector: (2D Flex Viewer Only) Opens the Cell Inspector window.

Linking 2D Viewer with Attributes Table

The 2D Viewer can be linked with the spreadsheet table such that when a polyline, polygon or point feature is selected in the 2D viewer, its corresponding attribute data is automatically highlighted in the spreadsheet table. Likewise, when an attribute row is selected in the spreadsheet table, its corresponding feature is highlighted in the active 2D Viewer. In order to have this bidirectional linking between viewer and spreadsheet table, the 2D Viewer must

be in Pick mode, and the spreadsheet table must be opened.



5.3.1 Cell Inspector

The Cell Inspector is available when a 2D view (i.e. Layer, Row, Column) is active in a Flex Viewer associated with either a <u>regular finite difference grid</u> or <u>unstructured grid</u> Numerical Model Workflow step.

Clicking the iso on will open a Cell Inspector for *the numerical model associated with the active workflow step.* The title bar of the Cell Inspector will include the name of the numerical to which it applies. You can open one cell inspector for each numerical model in your project. The Cell Inspector window consists of two tabs <u>Cell Values</u> and <u>Select Items</u>.

Cell V	alues	
Group View	List View	Select Items

			C	Cell V	alues	5							
Group View					List View						Select Items		
cel	I Inspector (SEA)	VAT-Run1)	- 0	x ı	Cell Ins	pector (SEAWA	T-Run1)	_		\times	🔯 Cell Inspector (SEAWAT-Run1) — 🗆	>	
ell valu	es Select items				Cell values	Select items					Cell values Select items		
G	oup view	- + 1 🔳	Time: 0		🛞 List vie	ew -	1 1 🔳 🖗	Time: 0			🛞 🗍 🐒 🗆 🕰 🔍 Search		
Po	sition			^	Group V	Name	V Object V	Value 🛛	Unit 🔽	~	Position		
ė	SEAWAT				Position	Layer	SEAWAT	23			🖻 🗹 SEAWAT		
	Layer	23			Position	Row	SEAWAT	1			- 🔁 Layer		
	Row	1			Position	Column	SEAWAT	53			Row		
	Column	53			Position	ModelX	SEAWAT	525	m				
	ModelX	525	m		Position	ModelY	SEAWAT	100	m		ModelX ModelY		
	ModelY	100	m		Position	ModelZ	SEAWAT	-225	m				
	ModelZ	-225	m		Position	WorldX	SEAWAT	525	m		WorldX		
	WorldX	525	m		Position	WorldY	SEAWAT	100	m	-			
	WorldY	100	m		Position	WorldZ	SEAWAT	-225	m		WorldZ		
	WorldZ	-225	m		Properties	Кх	Conductivity1	10	m/d		Properties		
Pro	operties				Properties		Conductivity1	10	m/d		Conductivity1		
ė	Conductivity1				Properties	Kz	Conductivity1	0.1	m/d		- ∠ Kx		
	— Kx	10	m/d		Properties	Zones	Conductivity1	1			- 🗹 Ky		
	— Ку	10	m/d		Properties	Sy	Storage1	0.2					
	- Kz	0.1	m/d		Properties	Ss	Storage1	1E-05	1/m		Zones		
	Zones	1			Properties	Ep	Storage1	0.35			⊖ Ø Storage1		
ė	Storage1				Properties	Тр	Storage1	0.35			- ⊠ Sy		
	- Sy	0.2			Properties	Zones	Storage1	1					
	Ss	1E-05	1/m		Properties	InitialHeads	Initial Heads1	0	m				
	- Ep	0.35			Properties	Zones	Initial Heads1	1			Zones		
	— Tp	0.35		~	Properties	Zones	Salt	1		~	Initial Heads1		

Cell Values Tab

The Cell Values tab displays the values (in group view or list view, see table above) for selected items applicable to the most-recently queried cell in the relevant model.

Values in the Cell Values tab are read-only and cannot be modified. The one exception to this is are cell address value(s). For finite difference grids the cell address consists of the Layer, Row, and Column indices (i,j,k), while in unstructured grids, the cell address consists of a single global cell index (i). Editing these values will refresh the Cell Values tab with the values associated with the newly entered cell address.

Controls

The following controls are part of the Cell Values tab:





Refresh: re-queries the values based on the current cell address.

View Type: Allows you to select either group view or the list view. The group view is the default view and presents cell data in

hierarchical groups (e.g. Input > Conductivity > Kx). The list view presents all information in tabular format with each hierarchic level given its own field and facilitates copying the data to external formats (such as spreadsheets).

Expand All: Allows you to expand all grouped nodes in the Cell Values Tab

Collapse All: Allows you to collapse all grouped nodes in the Cell Values Tab

Select All: Allows you to select all values in the Cell Inspector Cell Values Tab

Copy Selection: Allows you to copy the selected cell(s) to the Clipboard for pasting the selected values into an external application (i.e. spreadsheet or text editor)

Time Indicator: Indicates the time step/stress period applicable to the cell inspector and is based on the value shown in the time picker for the active view. Times are shown in relative time

Select Items Tab

The Select Items tab allows you to select which model items (e.g. grid properties, model properties, or boundary conditions) will be displayed in the values tab.

Controls

The following controls are part of the Cell Values tab:

8 .	1100	Search	\mathcal{R}
8	Refresh : refreshes all d adds/removes groups b boundary conditions, ar	ased on newly created	•
1	Expand All: Allows you items Tab	to expand all grouped	I nodes in the Select
î	Collapse All : Allows yo items Tab	u to collapse all group	ed nodes in the Select
đ	Select All: Allows you to	o select all model data	i nodes
	Select None: Allows yo	u to clear all selection	S
1	Show Selected: Allows hide the deselected iten	· ·	selected items and
Q	Show Deselected: Allo and hide selected items	,	ne deselected items
Search	Search: Allows you to ty items	ype text that will be us	ed to search and filter
\mathbb{R}	Clear Search: Allows to items	clear the search and/	or show all hidden

5.4 Adjusting Viewer Settings

The following settings are available in both 3D and 2D Viewers:

- Changing the Background Color: To change the background color of a 2D or 3D Viewer, right-click anywhere within the viewer, and select Background Color from the pop-up menu. The Color combo box will display on your screen. Select a new color and then click the [OK] button.
- Showing the Viewer Axis: To show or hide the viewer axis, right-click anywhere within the viewer, and select Axis from the pop-up menu.

The following settings only apply to 3D Viewers.

- Setting the Vertical Exaggeration: The Vertical Exaggeration is the ratio of the scale of the Y-axis to the scale of the X-axis. Vertical exaggeration can be used for discerning subtle topographic features or when the data covers a large horizontal distance (miles) relative to the relief (feet). By default, the vertical exaggeration is set to 0. You can change the vertical exaggeration using the Exaggeration text box, located at the bottom of the 3D Viewer (shown below).
- **Resetting the Viewer**: To zoom out to the full extents of your data click the Reset Scene Position button located at the bottom of the viewer.

Please Note: clicking this button will reset the rotation and zoom level back to the original view configuration.

3D Viewer - Creating Cutaways

Visual MODFLOW Flex allows you to remove portions of the model from the 3D Viewer by creating cutaways. To create a cutaway in a 3D-Viewer, follow the steps below:

CutAway Pro					
YZ Slice ☑ Active	leftright	X Position 489647.382	Xmin 481897.382	Xmax 497397.382	Fraction 0.5
XZ Slice	● before ○ after	Y Position 4874380.309	Ymin 4867005.309		Fraction 0.5
XY Slice	aboveunder		Zmin 78.51826256	j i	
			Apply	ОК	Cancel

- Right-click anywhere inside the 3D Viewer, and select CutAway Properties from the pop-up menu. The following dialog box will display on your screen.
- Click the CutOffs Active check box to enable CutAways.
- Under the Activity tab, specify which slices to make active by clicking the appropriate Active check boxes. The YZ slice refers to a vertical plane along the Y and Z axis, the XZ slice refer to a vertical plane along the X and Z axis, and the YZ slice refers to a horizontal plane along the Y and Z axis.
- For each active slice, select which portion to remove from the viewer (for example, the portion of the model that is left or right side of the slice, before or after the slice, or above or under the slice).
- By default, the position of each slice is automatically positioned in the middle of the data along its respective axis. However, you can manually change the position of the slice by entering a new value in the Position field.

Please Note: the Xmin, Xmax, Ymin, Ymax, Zmin and Zmax fields are read-only, and cannot be changed.

- Alternatively, you can set the position of a slice by entering a value in the Fraction field. For example a fraction value of 0.5 will set the slice position in the middle of the 3D data.
- Click the [OK] button to apply the changes to the current 3D Viewer.

3D Viewer Performance Preferences

For details on adjusting the 3D View performance settings, see <u>3D Viewer Preferences</u>.

5.5 3D Viewer Animations

The 3D Viewer can animate items and also record static or transient models to .AVI file.

Right-click on the 3D viewer and select the Animation Parameters. The following options are available:

Animation Parameters	– 🗆 X
🗹 Rotate 🗌 Transient Time	Time Delay (ms)
Rotate Time	
Rotate on X-axis	
Rotate on Y-axis	
Rotate on Z-axis	
Video	
Write Video File	
C:\Files\video1.avi	
Resolution	Compression
1920*1080 ~	Stardard Quality Video (70) $$
	OK Cancel

Rotate will allow you to rotate the model domain around the specified axis.

If you wish to save to a video file, select the check box beside Write Video File and specify a name and directory. The combo box below this allows you to specify the video resolution.

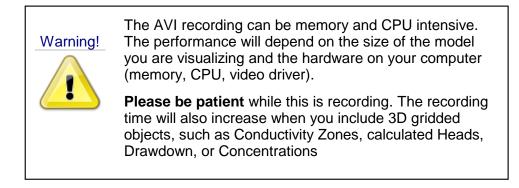
If you click on the Time tab, you will have options to specify the start and end time and the number of time frames. These options are only appropriate if you are animating Heads or Drawdown that has multiple output times.

Animation Parameters – 🗆 🗙						
☐ Rotate	ne Time Delay (ms) 200					
Start Time 0.00 End Time 3650 Frames 365	Min Time: 0.00 Max Time: 3650 Time steps: 365					
Video Write Video File C:\Files\video1.avi Resolution 1920*1080	Compression Stardard Quality Video (70)					
1320 1000	OK Cancel					

Click OK after defining the desired Animation settings.

Then right-click on the 3D viewer and select Animate and the rotation will start. If you have selected to record a video file, then the video recording will begin.

Once you are done recording, right click on the 3D viewer again and select Animate to stop the animation.



5.6 Exporting Views

To export a 2D Viewer to a graphics file, e.g., *.BMP, .*TIF, *.GIF, *.JPEG, follow the steps below:

- Right-click anywhere within the viewer
- Select Export Current View to Image from the pop-up menu.
- A Save As window will display, allowing to you specify the location on your computer where the graphics file will be saved.

To export a 3D Viewer to a graphics files, follow the steps below:

- Right-click anywhere within the viewer
- Select Save as image from the pop-up menu.
- The following dialog box will display on your screen:

🐯 Save as I	mage		_		\times
lmage Size Width	3200 * 2400	Height		~	
File Name White Back	ground Color 🗹				
		OK		Cance	

- Select the desired image size from the Image Size combo box. If you select Custom, then specify the desired image dimensions in the Height and Width combo boxes.
- Click the [...] button and specify a folder location on your computer to save the image file.
- Click the [Ok] button to save the image.

6 Data Settings

Visual MODFLOW Flex allows you to view and modify various settings and properties for each imported or digitized data object. In general, data object settings consist of the following categories:

- **General**: View data object metadata including source data information, statistics, native coordinate system, field mappings; view the attribute and geometry table.
- **Operations**: Apply arithmetic and geometric operations to data object geometry and attributes.
- **Style Settings**: Modify various style settings for different data object elements, e.g., point/line symbology, show labels, color rendering by attribute, create isosurfaces, set transparency etc.

Data object settings can be accessed from the main Visual MODFLOW Flex window. To view the settings for a data object, in the Data Explorer, right-click on the desired data object and select Settings... from the pop-up menu.

airport-laye airport-laye airport-laye	-
	View Spreadsheet Export Delete Import Data Create Surface Create New Data Object New Folder
	2D Viewer 3D Viewer

This chapter presents information on the following topics:

- Viewing <u>General Settings</u>
- Viewing the Data Table
- Performing Data Operations
- Modifying <u>Style Settings</u>

6.1 General Settings

General settings consist of data object meta data including the coordinate system, field mappings, and source data information. General settings can be accessed by expanding the General node in the Settings tree. The settings in each sub-node are described below.

Title Bar

The title bar of the General Settings window will include the name of the data object and the viewer in which the style settings apply.

	BJECT APPLICABLE VIEWER
😂 Settings - Boundary	
Settings - boundary	
General	Info
···· Info ···· Details	Name
Statistics	Boundary Table
	Туре
	Polygon
	Data Source C:\Files_Flex\Projects\Mildmay\Inputs\Snapped\boundary_s.shp Color Description
	Apply OK Cancel Help

Info

The Info node contains the following information:

- Name: The name of the data object (read only) defined during import.
- **Type**: The type of the data object, e.g., points, polygon, polyline.
- Data Source: The folder path of the data source when the data was imported.
- **Color**: The color of the data object when displayed in 2D and 3D Viewers. Click the color box to select a new color for the data object.
- **Description**: The description of the data object as defined during import. This field is editable allowing you to update the description at any time.

Table (Button):The table button allows you to view the geometry and attributes of the data object in a table view. For more information on the table view, please see "<u>Viewing the Data</u> <u>Table</u>" section.

Details

The Details node contains information on the coordinate system of the data object, and the field mappings specified during import.

Statistics

The Statistics node displays a count summary of the various data elements that comprise the data object. For example, for polygon data objects, the statistics node will show the number of polygons, polygon parts and vertices in the data object. For cross section data objects, the number of wells and cross sections is displayed.

For Property and Structural Zone conceptual model objects, various statistics are automatically calculated and displayed under the statistics nodes, including: Min and Max X, Y and Z values, Area and Volume.

6.2 Data Operations

Visual MODFLOW Flex allows you to apply various operations that modify the elevation or attribute data of objects in the Data Explorer. Operation settings can be accessed by clicking on the Operations tree node in the Settings window. (To access the Settings window, in the Data Explorer, right-click on the data object and select Settings... from the pop-up context menu).

🐯 Settings - Streams (2	D Viewer - 1)				×
	Arithmetic				
Operations Arithmetic Style	Select Operation				
	Z = Constant				\sim
	Description and Instructions				
	For all Z-values in the object, apply	Z = Constant. Assign the values from (Constant.		
	Input Parameters				
	Parameter	Value			
	▶ constant				
	Save As New Data Object			Execute	
		Apply OK	Cancel	Hel	p

Scope

Visual MODFLOW Flex supports the following types of data operations:

- Arithmetic Operations: Polygons, Polylines, Points, Surfaces, and Maps only
- Attribute Operations: Surface, Points, Time Schedules only
- Data Conversion Operations
- Converting Well Tops to Points Data: Wells Objects only

Each type of operation is described in detail in the sections below.

Arithmetic Operations

Arithmetic operations allow you to alter the elevation values of features in the selected data object based on a user-specified arithmetic expression using the <u>Expression Builder</u>. For example, you can use this option to drape a map over a specified surface data object. You can also shift the elevation of polylines, polygons, points or surfaces up or down by a specified constant value. Arithmetic operations can be applied to polygons, polylines, points, surfaces, and maps.

When the Arithmetic node	is selected from the	e Settings tree, the	following dialog	y will display:

🐯 Settings - Model Bo	undary (3D Viewer-1)		— 🗆 X
⊕. General	Arithmetic		
i - Operations i Arithmetic	Variables & Constants	Data Objects SurfaceBaseBot1Bot1aBot2Bot2aPinched 2PinchedSurface 30Surface 60Top1WTWTWT	Functions abs average cif cos dot exp ifgaps In log log10 max min mod mult not pmax pmin round sigdig sin sqrt sum tan
	+ - × Expression Elevation Save As New Data O		Execute
		Apply OK	Cancel Help

To apply an arithmetic operation follow the steps below:

• Select the desired arithmetic expression from the Select Operation combo box.

- If you are unsure of what the expression does, refer to the provided description in the Description and Instructions text box.
- The contents of the Input Parameters frame will vary depending on the selected expression.
- If the selected expression contains a constant value, e.g., Z = Constant, enter a value in Value field.
- If the selected expression requires a surface, e.g., Z = Surface(x,y), then select the desired surface from the Data Explorer, and then click the button to insert the surface into the Value field.
- Optional: Select the Save As New Data Object check box to save the transformed data as a new data object.
- Click the [Execute] button to apply the operation.

Please Note: If the data object is being viewed in a 3D Viewer while the operation is applied, you may have to turn off the data object, and then turn it back on to see the changes.

Attribute Operations

The Attribute Operations settings pane allows you to modify attribute values for point, surface, and time schedule objects in the Data Explorer using an Expression. Note that point and surface objects are spatial in nature so they will include valid data objects such as surfaces and horizons; however, time schedule objects do not have a spatial component and surfaces/horizons will not be included in the Data Objects list.

😂 Settings - Streamflow		_	
General Operations Arithmetic Attribute Streamflow_co Variables & C Ifalse	s v	Functions	
pi streamflow_c true		abs average cif cos dot exp ifgaps In log log10 max min mod mult not pmax pmin round	~
Expression	+ - × ÷ () < >	= X ^y	
Save As N	lew Data Object		Execute
	Apply OK	Cancel	Help

To apply an attribute operation:

- Select the desired attribute to modify using the Attribute dropdown list.
- Enter a valid <u>expression</u> in the Expression form
- Optional: Select the **Save As New Data Object** check box to save the transformed data as a new data object.
- Click the **Execute** button to apply the operation

Context Menu Operations

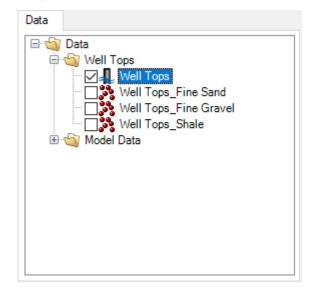
Certain operations can be performed directly on specific objects to convert these objects to a different type.

Converting Well Tops to Points Data Object

This operation allows you to create a new points data objects based on Well Top information. One set of points will be created for each listed formation in the wells data object. The resulting points data objects can then be used to create surfaces, which in turn can be used to define the horizons of a conceptual model.

Well top data can either be included during data import, or they can be manually defined in the well table view. For information on defining well tops, please see description of "<u>Well</u> <u>Tops</u>" in the Well Data table section.

To perform this operation, right-click on the desired wells data object in the Data Explorer, and select **Convert Well Tops to Points** from the pop-up context menu.



Once the points data objects are created, they are added to the same folder as the Well Tops object in the Data Explorer using the naming convention: [wells data object name] _[formation label], as shown above.

6.3 Style Settings

Visual MODFLOW Flex provides you with a wide variety of style settings, allowing you to modify the appearance of data objects in both 3D and 2D Viewer. The style settings can be accessed by expanding the Style node in the Settings tree (shown below).

Please Note: the Style node will only be available when the particular data object is being shown in a viewer.

In general, each data object has its own set of style settings, although some settings are common between data objects. The following sections describe the style settings for the various data objects.

General	Style	
⊕ Operations ⊖ Style - General ⊕ Labels - Colors	Appearance Color Specified Symbol Circle	
	Show Vertices Preview	
	•	

Select the links below to jump to the appropriate sections:

- Points, Polylines, and Polygons
- Cross-Sections
- Wells
- Surfaces
- 3D Gridded Data

6.3.1 Points, Polylines, and Polygons

Points/Vertices

The style settings for points data objects are described below:

General	General
Operations Style General Colors Tabels	 Show Vertices Appearance Color By Attribute Symbol Circle Size 2 Show in Cutaway region

Select the color method, symbol, and size from the appropriate combo boxes.

The Show in Cutaway check box allows you to show points or vertices in cutaway regions in the 3D Viewer window. When this option is disabled, points or vertices will not show in any areas that have been "hidden" in the 3D Viewer window by creating "Cutaways". For information on creating cutaways, please see "Adjusting Viewer Settings" section.

Choose from the following color methods:

- **Specified**: Points are colored using the color specified in the General settings.
- **By Attribute**: Points are colored based on a specified data object attribute as explained below.

Color By Attribute

Data objects can be colored based on a specified attribute. Color rendering can be applied to any shape element that contains attributes. To color a data object by attribute, follow the steps below.

In the Settings for the selected data object,

- Expand the Style node and select the shape element to be colored, e.g., Points
- From the Color combo box, select the By Attribute option.
- From the Settings tree, select the Colors node and the following dialog will appear.

	Colors			
Operations Style	Select Data			
General	Attribute		Max: 361.6556	
Colors	AvgWLevel	•		
Labels			Min: 244.9531	
	Color Classification			Max: 361.6556
	🔲 Use Proje	ct Color Palette	now Project Palette	
	Туре	Classes		
	Stretched	Number of Class	ses 7 🚔	
	Classified	Equal Intervals		
	Color	Value	Label	
	255, 0, 0	361.65562649291		
	250, 165, 1	342.205211039316		
	190, 255, 7	322.754795585723		
	91, 255, 49	303.304380132129		
	64, 255, 167	283.853964678535		
	44, 166, 240	264.403549224942		
	8, 8, 255	244.953133771348		
				2 - C
				Min: 244.9531
				Mill: 244.0001
		Apply	OK Cano	el Help

• Select the desired attribute from the Attribute combo box. You will notice that the min and max values are displayed to the right of the combo box. Some data objects will have attributes while others will not. The following table lists which data object types can have attributes available for color rendering:

Data Object	Available Attributes
Points, Polygons, Polylines	Only if attributes were created during import
Surfaces	Z

3D Gridded Data	Z and other attributes that were added during import
Conductivity	ZoneID, Kx, Ky, Kz
Storativity	ZoneID, Ss, Sy, Tp (total porosity), Ep (effective porosity)
Initial Heads	ZoneID, Initial Heads
Recharge	ZoneID, Recharge Rate, Ponding Depth
Evapotranspiration	ZoneID, Evapotranspiration Rate, Extinction Depth.
Heads	Head
Drawdown	Drawdown
Concentrations	Concentration
Velocity	

·

Gridded Input Data Available Attributes

Conductivity	ZonelD, Kx, Ky, Kz
Storativity	ZoneID, Ss, Sy, Tp (total porosity), Ep (effective porosity)
Initial Heads	ZoneID, Initial Heads
Recharge	ZoneID, Recharge Rate, Ponding Depth
Evapotranspiration	ZoneID, Evapotranspiration Rate, Extinction Depth.
Unsaturated Zone (UZF)	ZoneID,

Gridded Output Data	Available Attributes
Heads	Head
Drawdown	Drawdown
Budget	
Velocity	
Water Table	
Concentrations	Concentration

 Select the Color Classification: by default, the colors will be calculated from the min and max values for the current data object. Visual MODFLOW provides an option to use Project-wide Color Palettes. This is useful when you have multiple data objects that are rendering the same attribute (e.g. heads from different model runs, conductivity distributions), and you want to make qualitative comparisons between these. This is challenging when each data object has its own min and max values and are colored based on this. However this becomes much easier when these data objects all read from a common color palette. If this option is checked on, you can access the color palette and adjust min and max values. See <u>Project Color Palettes</u> for more details.

 For the selected attribute, you can define various settings. These settings are described below.

Type: Select between Stretched or Classified. The stretched option allows for color shading, i.e, continuous color gradient. The classified option allows for discrete intervals, i.e., zebra, in the color gradient.

Classes: There are two options for defining the number of classes to be used: Number of Classes and Equal Intervals.

Number of Classes: Specify the number of color classes in the text box.

Equal Intervals: Specify an interval spacing, and the number of classes will be determined from the range of the attribute data. For example if your data rage is 100, and you specify a 10 interval spacing, 10 classes will be created.

As the number of intervals/classes is modified, rows are automatically removed or added to the color table. For the Elevation color scheme, the maximum value will always be Red and the minimum value will always be Blue, but the gradient between will change automatically depending on the specified number of classes.

- Visual MODFLOW Flex automatically calculates the intervals based on the defined specified number of classes or equal intervals.
- Once the settings have been defined, click the [Apply] button to show the changes in an active 2D or 3D Viewer.

Area

Select the Show Area Fill check box to show/hide the area file. If unchecked, only the shape boundary will be visible in 2D and 3D Viewers.

. ⊕- General	General
🕂 Operations	
⊟- Style	
i i Area	
	Show Area Fill
General	I™ Show Area Fill
. to Labels	
Colors	Fill Settings
🗄 Lines	Color
	Specified
	Pattern
	VIII Up Diagonal
	Transparency
	0
	Preview

Select the color method and fill pattern symbology, from the appropriate combo boxes.

Choose from the following color methods:

- Specified: Shape is colored using the color specified in the General node.
- **By Attribute**: Shape is colored based on an attribute. See "Color By Attribute" section for more information on color rendering.
- **Custom**: Specify a color for the area fill. This color will overwrite the default color defined in the general settings for this particular shape element.

Select the Transparent checkbox to make the polygon fill pattern transparent. Use the adjacent Transparency text box to set the level of transparency, e.g., a higher value will make the fill more transparent.

The Show in Cutaway check box allows you to show areas the polygon in cutaway regions in the 3D Viewer window. When this option is disabled, the polygon will not show in any areas that have been "hidden" in the 3D Viewer window by creating "Cutaways". For information on creating cutaways, please see "Creating Cutaways".

Lines

Select the Color method, line Pattern (solid or dash), line Width from the appropriate combo boxes.

🛃 Settings	
Settings	General Show Lines Color Specified Type Type Type Type Type Type Type Type Type Type
	Width 1 Preview

Choose from the following color methods:

- **Specified**: Line is colored using the color specified in the General settings.
- **Custom**: Specify a color for the line element. This color will overwrite the default color defined in the general settings for this particular shape element.

The Show in Cutaway check box allows you to show areas the line in cutaway regions in the 3D Viewer window. When this option is disabled, lines will not show in any areas that have been "hidden" in the 3D Viewer window by creating "Cutaways". For information, please see the "Creating Cutaways" section.

Labels

⊕- General	General	
⊕ • Operations		
⊟- Style	Show Labels	
🖹 Lines		
General	Text String	
🖻 Labels	Label Field	
General		
- Format	WIDTH	▼
- Placement		
Colors		
Vertices	Text Symbol	
	Font	Size
	Arial	10 💌
	Style	Color
	Regular 💌	
	Preview	
	ABC	
	/B0	

General

The following label settings are available under the General node (shown above):

- Show Labels: Show/Hide the labels in 2D/3D viewer.
- Label Field: This combo box contains all attributes for the selected data object. Select the desired attribute field to use for the labels.
- Font: Select the label font from the combo box.
- Size: Set the text size of the labels.
- Style: Set the font style for the labels, e.g., Regular, Bold, Font, Italicized, etc.
- **Color**: Set the color of the label text.

Format

The following label settings are available under the Format node:

- Format: Choose between Numeric or Scientific notation.
- Decimals: Set the number of decimals to plot for each label.

Placement (Polylines only)

The following label settings are available under the Placement node:

- **Position**: Display the label above, below, or on the line.
- Offset: This parameter controls how far the label will be placed from the line.
- Location along the line: Display the label at the start, in the middle or at the end of the line.
- Orientation to the line: Display the label parallel, perpendicular or horizontal to the line.

6.3.2 Cross Sections

The following section describes the available style settings for cross-section data objects.

To access the style settings, right-click on the cross-section data object in the Data Explorer, and select Settings... from the pop-up context menu. Then, in the Settings dialog, expand the Style node to view the style settings.

😻 Settings - Site Cross S	Section	- D >	<
 General Operations Style Interpretation Wells 	Interpretation Interpretation Type Mode Show Labels Show All	~	
	Visible	Cross Section AA BB CC DD EE FF GG	
		Apply OK Cancel Help	

Cross-section data objects consist of two main elements; the interpretation layers and the cross-section wells. The settings for each element can be accessed by clicking on the Interpretation or Wells node, respectively.

Interpretation

A screen capture of the interpretation settings is shown above. From the Interpretation Type combo box, select which interpretation layer to show in 3D Viewer. Select from Model, Geology or Hydrogeology.

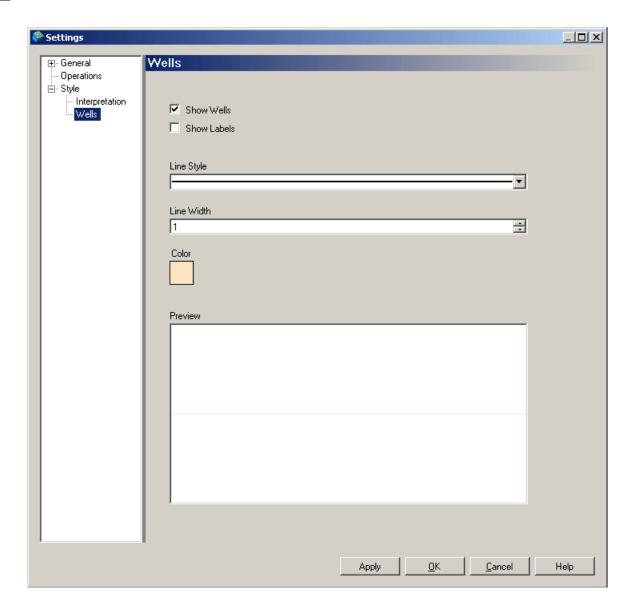
When an interpretation layer is selected from the combo box, its associated cross-sections are listed in the grid below. Under the Visible column, select which cross-section to show/hide in 3D Viewer.

Select the Show All check box to show all the cross-sections for the selected interpretation layer.

Select the Show Labels check box to show the label for each cross-section.

Wells

The wells node contains settings for changing the appearance of the cross-section wells. These settings are described below.



- Show Wells: Check this option to show the well geometry.
- Show Labels: Check this option to show the well label above each well.
- Line Style: Select the type of line to display. Choose between solid or dashed.
- Line Width: Specify the width of the wells.
- Color: Change the color of the wells.

Click the [Apply] button to display the changes in an active 3D Viewer window.

6.3.3 Wells

The following section describes the available style settings for Wells data objects.

To access the style settings, right-click on the well data object in the Data Explorer, and select Settings... from the pop-up menu. Then, in the Settings dialog, expand the Style node to view the style settings. There are several different style settings that will be shown depending on whether the Wells set is a data object in the Data Explorer or the Model Explorer.

Well Heads, Well Tops, and Observation Points

The well heads, well tops, and observation points (obs.point) subnodes provides settings for the 3D points representing:

- Well Head: the top elevation of the well casing.
- Well Tops: top elevations of interpreted hydrostratigraphic model layers along the well path(s)
- **Obs.Point**: the point(s) along the well path(s) representing observations to be used for model analysis and calibration/history matching; typically the midpoint the well screen(s) or the bottom elevation of piezometer(s)

General Settings

When the General subnode is selected, the following options are available:

😻 Settings - Well 4 (K	INCARDINE_NORTH grid-Run/BoundaryConditions/3D View)	_		×
Settings - Well 4 (K ⊕ General ⊕ Syle ⊕ Well Tops ⊖ Colors ⊕ Labels ⊕ Well Path ⊕ Screens ⊕ -Cells ⊕ Time	INCARDINE_NORTH grid-Run/BoundaryConditions/3D View) General Show Appearance Color Custom Symbol Circle Size 2 Show in Cutaway region Show in Cutaway region			×
	•			
	Apply OK	Cancel	Не	p

- Show: Select this option to show/hide the well tops.
- Color: Select a color the well tops.
- **Symbol**: Select the well head symbology from the combo box. Choose from various symbols including circle, square, cross, diamond etc.
- Size: Specify the size of the well tops.

Click the [Apply] button to view the change in an active 2D or 3D Viewer.

Colors

For more information on the Colors node, please see the "Colors" section.

Labels

For information on the Labels node, please see "Labels" section.

Well Path

The Well Path subnode provides options for changing the appearance of the well path. These options are described below.

General

When the General subnode is selected, the following options are available:

- Show Lines: Select this option to show/hide the well path.
- Color: Select a color the well paths.
- **Type**: Specify the line type for the well path. Choose between a solid line or a dashed line.
- Width: Specify the width of the well paths.

Click the [Apply] button to view the change in an active 2D or 3D Window.

Well Screens

The Well Screens subnode provides options for changing the appearance of the screens along the well path. These options are described below.

Settings - Well 4 (Kl	NCARDINE_NORTH grid-Run/BoundaryConditions/3D View)			\times
	General			
B: Style B: Weil Tops B: Weil Path D: Screens Colors B: Vertices B: Cells B: Time	Show Lines Color Custom Type Type Type Type Type Type Type Type			
	Apply OK C	Cancel	Help	

When the General subnode is selected, the following options are available:

- Show Lines: Select this option to show/hide the well screens.
- Color: Select a color for the well screens.
- **Type**: Specify the line type for the well screens. Choose between a solid line or a dashed line.
- Width: Specify the width of the well screens.

Click the [Apply] button to view the change in an active 2D or 3D Window.

Colors

For more information on the Colors node, please see the "Colors" section.

Screen Cells

The cells subnode provides options for displaying the model cells that intersect the well screens. These options are described below.

General

When the General subnode is selected, the following options are available:

🐯 Settings - Well 4 (KIN	CARDINE_NORTH grid-Run/BoundaryConditions/Column View)	_		×
Settings - Well 4 (KIN General Syle Well Tops Well Path Screens Screen Cells Area General	General Show Area Fill Fill Settings Color Custom Pattern Solid Transparency			×
	Solid ~			
	Apply OK Ca	ancel	Help	2

- Show Area Fill: Select this option to show/hide the cell areas.
- Color: Select a color for the cells
- **Pattern**: Select the pattern from the combo box. Choose from various patterns including solid, horizontal (lines), vertical, diagonal, etc.

Click the [Apply] button to view the change in an active 2D or 3D Window.

6.3.4 Surfaces

The following section describes the available style settings for Surface data objects.

To access the style settings, right-click on the surface data object in the Data Explorer, and select Settings... from the pop-up menu. Then, in the Settings dialog, expand the Style node to view the style settings.

Colors

⊕ General	Colors	
⊡ ·· Operations ⊡ ·· Style Colors	Show Color Fill	Show Legend
Contour Line	Select Data Attribute Z	Max: 21.20000 Min: 16.51553
	Transparent	%
	Use Project Color Palette	Show Project Palette
	Туре	Classes
	 Stretched Classified 	Number of Classes Section 2015 Section 2015
	Color	Value
	255, 0, 0	21.2
	255, 146, 0	20.53079
	227, 255, 3	19.86158
	118, 255, 15	19.19237
	64, 255, 83	18.52316
	64, 255, 208	17.85395
	40, 149, 246	17.18474 16.51553
	0, 0, 200	16.01000
		Min: 16.5155

The Colors node provides options for coloring the surface layer by elevation value. The following options are available:

- Show Color Fill: This option allows you to show or hide the color fill. If disabled, the surface will appear in the color defined in the General settings.
- **Transparency**: This option allows you to make the surface appear transparent. When the Transparent checkbox is selected, use the adjacent slider bar to set the level of transparency.
- **Type**: Select the type of gradient to use for coloring the surface. Select Stretched to use a continuous color gradient, or select Classified to use discrete color zones.
- **Classes**: There are two options for defining the number of classes to be used: Number of Classes and Equal Intervals.

- o Number of Classes: Specify the number of color classes in the text box.
- *Equal Intervals*: Specify an interval spacing, and the number of classes will be determined from the range of the attribute data. For example if your data rage is 100, and you specify a 10 interval spacing, 10 classes will be created.

As the number of intervals/classes is modified, rows are removed or added to the color table. The maximum value will always be Red and the minimum value will always be Blue, but the gradient between will change automatically depending on the specified number of classes.

Click the [Apply] button to view the changes in an active 2D- or 3D-Window.

Contour Lines

💭 Settings - Heads		- D X
General	Contour Lines	
È. Style Colors Contour Lines	 Show Contour Lines Heads Show Contour Labels Automatic contour Contour Interval 5 Start Contour Value 310 Finish Contour Value 370 	Min Value 313.055694580078 Max Value 361.706970214844 Custom Contour Use Custom Contour Levels New Value Add New Remove
	Lines style settings Line Style Line Width 1 Color Custom	Label settings Label Spacing 100 Label Margin 1 Number of decimals: 2 Label Font
	Apply	OK Cancel Help

The Contour Lines node provides options for showing contour lines on the surface layer. The following options are available:

- Show Contour Lines: Show/Hide the contour lines.
- Show Contour Labels: Show/Hide the contour labels.
- Contour Interval: Set the contour increment value.
- Start Contour Value: Value above which automatic contours will be displayed
- Finish Contour Value: Value below which automatic contours will be displayed
- Use Custom Contour Levels: Show/Hide the custom contour values specified in the Custom Contour List window
 - o New Value: Value to be added to the Custom Contour List window
 - *Add New*: Add the "New Value" to the Custom Contour List window. Specified values must be within the range of the active dataset.
 - o Remove: Removes the highlighted value from the Custom Contour List window
- Line Style: Select the contour line style from the combo box. Choose between solid line or dashed line.
- Line Width: Set the width (thickness) of the contour lines.
- Label Spacing: Set the spacing between the contour line and the label.
- Number of Decimals: Set the number of decimals to show in the contour labels.
- Label Font: Select this button to specify the font settings for the contour labels.

Click the [Apply] button to view the changes in an active 2D or 3D Viewer.

6.3.5 3D Gridded Data

The following section describes the available style settings for 3D-Gridded data objects. These are objects that are tied to a numerical grid, such as properties (e.g. conductivities), boundary conditions (e.g. rivers), and outputs (e.g. heads, velocities, etc.), as well as the grid itself.

To access the style settings, right-click on the surface data object in the Data Explorer, and select Settings... from the pop-up menu. Then, in the Settings dialog, expand the Style node to view the style settings.

Cells

The Cells node allows you to specify style settings for the grid cells.

🐯 Settings - Heads (Nu	🕏 Settings - Heads (NumericalGrid-Run11/ModelRunResult/3D View) 📃 🗌				
Settings - Heads (Nur General General Colors Colors Colors Colors Slice Color Map Color Map Slice Color Map Slice Color Map Three Slices Three Slices Three Slices Three Slices Three Slices Three Slices Three Slices Three Slices Three Slices Three Slices	mericalGrid-Run11/ModelRunResult/3D View) General Show Cells View Vitual grid Fill Settings Color By Attribute Transparency 0 Show only Active Zone Show Legend Show only Borders	- -			
	Show in Cutaway	ancel	Help		

The Show Cell check box allows you to show/hide the grid cells in the 3D gridded data object. When the check box is selected, you can choose how to show the cells in the Color combo box in the Fill Settings frame. With the Specified option, select the adjacent color swatch and select the desired color to fill the cells. If you select Color by Attribute, you can color each cell according to a specified attribute, e.g., heads. Color by attribute settings can be defined by selecting the Color node, located under the Cells node.

For more information on the color by attribute feature, please refer to "<u>Color By Attribute</u>" section.

The Show only Active Zone check box allows you to show/hide inactive grid cells.

Vertices, Lines

For information on the settings available in the Vertices and Lines nodes, please refer the <u>Points \ Vertices</u> and <u>Lines</u> respectively.



	General				
yle ⊡Cells	Show Slice	Use virtual grid			
·· Lines ·· Vertices	Slice Settings	_			
Slice	Slice Type	Auto Apply			_
<mark>General</mark> Colors	Row			~	
Legend	Row Number (159)		1	÷	
Color Map solines					
hreeSlices oSurface					
ne					
	Fill Settings				
	_			~	
	Fill Settings By Attribute			~	
	_			~	
	By Attribute			~	
	By Attribute Transparency			~	
	By Attribute Transparency 0				
	By Attribute Transparency			~ Wireframe	
	By Attribute Transparency 0				
	By Attribute Transparency 0				
	By Attribute Transparency 0				
	By Attribute Transparency 0				
	By Attribute Transparency 0				

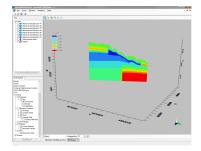
Show Slice will control the display status in the 3D Viewer.

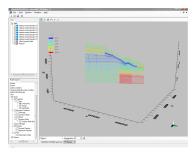
Use Virtual Grid option allows you to use a coarsened version of the true 3d grid dimensions. This option is recommended when you have moderate to large size grids (exceeding a few hundred thousand cells). If you have a small grid then this option can be turned off. For more details, see <u>Virtual Grid Settings</u>.

- Under Slice Settings, specify the desired Layer, Row, or Column Number.
- Under Fill Settings, the "By Attribute" option is default and recommended for most cases.
- Show Legend check box at the bottom of the window will add a color legend to the current 3d view
- Show Wireframe will render with wireframe instead of filled in cells. The example below illustrates this:

Filled Slice

Wireframe





In the Settings tree, under Slice > Colors, you can access the color page where you can choose which attribute you want to render; in the case of Properties (or Recharge and Evapotranspiration) you can render by Zone or by the specified Attribute (e.g. Kx, Recharge rate, etc..)For more information on the color by attribute feature, please refer to "Color By Attribute" section.

Colormap

Settings for the Colormap are identical to those explained above for Slice.

Gene	eral				
ls es tices	Show Colormap	🗹 Use virtua	al grid		
	map Slice Settings				
or Map	: Jype	Auto Appl	y		
Colors Rov					``
Legend					
nes eSlices	Row Number (159)			1	-
face					
Tran	ettings sparency				
	-	<u>÷</u>			
Tran 0	sparency			Uireframe	
Tran 0	sparency Show Legend				
	sparency Show Legend Use Upper Cutoffs	\$	Upper Cut Level	0	
	sparency Show Legend				

Plot Color Map on Cross-Sections

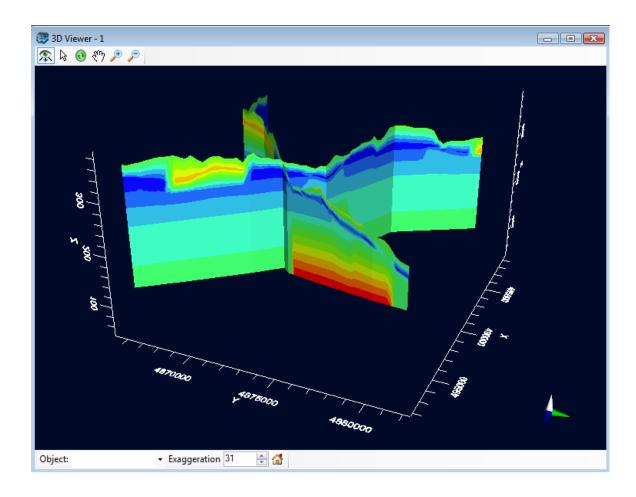
Color map has an additional **Slice Type**, which is "Cross Section", as shown below:

Settings	
General Style Cells Cells Colors Colors Colors Sources Sources Sources Sources Sources Sources Sources Sources	General Show Colomap Colomap Slice Settings Slice Type CrossSection
	Cross Section Polyline 1

After selecting this Slice Type, you need to provide a polyline data object that contains one or more polylines representing the cross-sections you want to render. Polylines can be imported from a shapefile or DXF file, or created manually. See <u>Creating New Data Objects</u> for more details.

Select this polyline data object from the tree, then click on the 📄 to insert this into the field as shown above.

Click Apply and the display will update with the appropriate cross-section lines. An example for two cross-sections is shown below.



In the Settings tree, under Colormap -- Colors, you can access the color page where you can choose which attribute you want to render; in the case of Properties (or Recharge and Evapotranspiration) you can render by Zone or by the specified Attribute (e.g. Kx, Recharge rate, etc..). For more information on the color by attribute feature, please refer to "Color By Attribute" section.

Isolines

Settings for the Isolines are identical to those explained above for Slice.

🐯 Settings - Heads (Numer	icalGrid-Run11/ModelRunResult/3E) View)	- 🗆 ×
	eneral		
⊡. Style ⊕. Cells ⊕. Lines	Show Isolines	Use virtual grid	Show Labels
enes enes	Isolines Slice Settings Slice Type		Auto Apply
En Color Map ⊡ Isolines	Row		~
General Colors	Row Number (159)	1	•
iter ThreeSlices iter IsoSurface iter Time	•		
	Select Data Attribute	Max: 383.52	
	Heads	Min: 275.07	
	Line properties Labels Custom Cor	ntour	
	Color	Number of contou	
	Specified ~	Contour Interval	T
		10.84	
	Line Width	Start value 275.07	
	·	Finish value	
	Use Start and Finish Values	383.52	
		Apply OK	<u>C</u> ancel Help

Isolines also has an option to plot on a Cross-Section; see <u>Colormap on Cross Section</u> as described above.

Under Select Data, choose the attribute you want to use for calculating Isolines: For Properties, you can choose from Zones or Attributes (e.g. Kx).

Additional Settings for Line Properties allow you to adjust the Line color, style, width. And, the number of contour lines, or the contour interval, and the starting value (minimum) by which contour intervals will be calculated. Settings in the Labels tab allow you to adjust the font size and color and the decimal format.

In the Settings tree, under Isolines -- Colors, you can access the color page where you can choose which attribute you want to render; in the case of Properties (or Recharge and Evapotranspiration) you can render by Zone or by the specified Attribute (e.g. Kx, Recharge rate, etc..). For more information on the color by attribute feature, please refer to "<u>Color By Attribute</u>" section.

Isosurfaces

The IsoSurface node allow you to create and modify one or more isosurfaces from 3D gridded attribute data. An isosurface is a 3D planar surface defined by a constant parameter value in 3D space. Isosurfaces are typically used for demonstrating the spatial distribution of a selected parameter. For groundwater modeling purposes, isosurfaces are generally used for representing the spatial distribution of heads, drawdowns, and concentrations.

ral	General		_		
ells nes	Isosurfaces	Show Isosurfaces	Use virtua	l grid	
ertices ice	Attribute	Value	Visible	Style & Color	
olor Map olines hreeSlices oSurface General Legend me	▶ Heads	350		ByAttribute	
	Add/Change Isosurface	Heads		-	
	☑ Show Legend	Add	Ch	ange R	lemove

Creating an Isosurface

To create an isosurface, follow the steps below:

- From the Attribute Name combo box, select the attribute from which the isosurface is to be created.
- Specify the attribute value in the Attribute Value field.

- Select the color method from the Color box. The isosurface can be displayed as a solid color (Custom) or rendered by a specified attribute (ByAttribute).
- Use the Visible check box to show/hide the isosurface.
- Use the Show Border check box to display/hide a color map of the element value on the borders (sides) of the model domain when the isosurface intersects the edge of the model domain.
- Use the Show in Cutaway check box to make the isosurface visible/invisible in cutaways.
- Use the transparent check box to enable/disable transparency. If enabled, use the Transparency slider to set the level of transparency/opaqueness.
- Click the [Add] button to create the isosurface.

The isosurface will be added to the isosurface table.

Modifying an Isosurface

To modify an existing isosurface, follow the steps below:

- Select the isosurface from the isosurface table.
- Make the modifications to the desired settings, e.g., attribute name, attribute value, color, etc.
- Click the [Change] button to apply the changes.

⊕ General	General
⊡·· Style ⊕·· Cells ⊡·· Time General	Show Time Label
	Transient Attributes Time Schedule
Slice Colomap isolines isosurfaces	1.0000 730.00 1460.0 2190.0 2920.0
 Busurfaces Three Slices 	3650.0 5475.0
	Font Size
	Font Color
	Time Label Style O Date Time (days)

Time

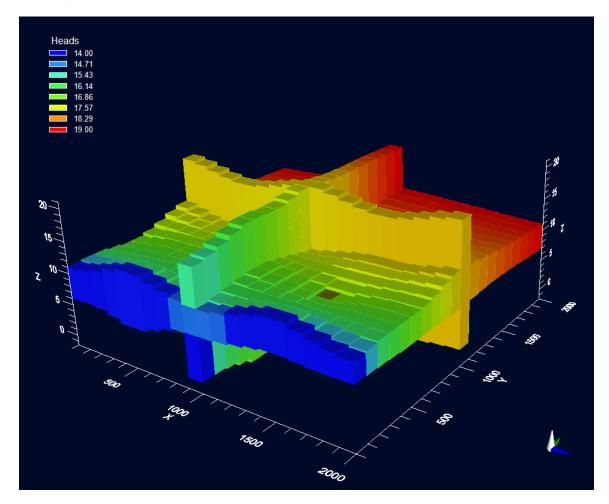
The Time node provides a list of all the time steps in the 3D gridded data object, and allows you to select the desired time step data to display in the 3D Viewer window. For 3D gridded data objects generated by steady state flow models, only one time step will be available. For 3D gridded data objects generated by transient flow models, multiple time steps will be available (as defined in the Translation settings in VMOD Flex, i.e, Translation / Time Steps).

ThreeSlices

seconds include (nume	ricalGrid-Run11/ModelRunResu				×
	eneral				
General General Style General Ge	Show Slice Wireframe Presentation Style Cells Layer (1-6)	3	Use virtual grid AutoApply		
	Column (1-62)	1	-		
	 Show Legend Use Upper Cutoffs Use Lower Cutoffs 		0		
		Apply Of	Cancel	Hel	p

The ThreeSlices option allows you to see a slice through a selected model layer, row, and column at the same time in the 3D view. This is the display option that is used when you view 3D Gridded objects in the 3D View of the Flex Viewer. An example is shown below,

with a slice through layer 2, and the center-most row and column in the Airport Transport tutorial project.



The generic options for "Slice" apply to the ThreeSlice including the Wireframe and "Use virtual grid" option.

The Colors and Legend options under ThreeSlice are also the same as described in earlier sections for Slice

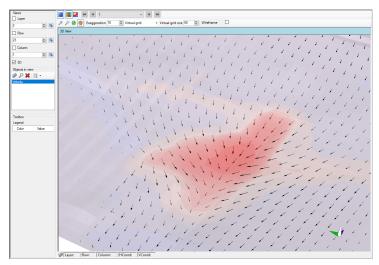
The following options are unique to ThreeSlice:

- Presentation Style: Choose between Cells and Surface; when Surface is selected, you will see a color map with Isolines; under the Isoline node in the Settings tree, you can adjust the contour interval and line style.
- Below Presentation Style, select the desired Layer, Row, and Column number for the slice.

VelocityMap

(Only available for output velocities)

The VelocityMap settings are only available for output velocities and allow you to visualize output velocities in a variety of ways.



General

Groundwater velocities can be shown along a specified row, column, and/or layer as directed vectors along the plane with options for the arrow lengths:

- Show: if selected, velocities will be displayed using the options described below
- Show normal velocity color map: if selected, velocities perpendicular to the selected viewing planes (row, column, and layer pickers) will be displayed as a color map using the options on the next tab (see <u>below</u>).
- Show isolines: if selected and the normal velocity color map is also selected, isolines for the perpendicular velocities will be displayed using the intervals on the colormap options on the next tab (see <u>below</u>).
- Color:
 - o Custom: velocity vectors will be displayed in the specified color selected on the right
 - By normal velocity: velocity vectors will be based on the flow perpendicular to the selected plane using the color options on the next tab (see <u>below</u>).
- Velocity Type:
 - Darcy: velocities are derived by interpolating inter-cell fluxes across the cell interfaces
 - Average Linear. average linear velocities (also called seepage velocities) are estimated by dividing the Darcy velocity by the effective porosity
- Show Vectors as:

- o Direction: View flow direction vectors (not-to-scale velocity vectors)
- o *Projection*: View projections of the velocity vectors onto the current plane of view.
- Magnitude: View velocity vectors scaled according to the magnitude of the flow velocity in any direction.
- Scale:
 - o Linear: velocity vectors are scaled by the linear value
 - o Logarithmic: velocity vectors are scaled by the logarithmic value
- Scale Factor: velocity vectors are scaled by the specified value

😂 Settings - Velocity (Nu	_		×	
⊕. General	General			
	Show Show legend Show normal velocity color map Show isolines Show layer 3 Show row 36 Show column 30 Velocity Vectors On X 29 On Y 29 On X 29 On X By normal velocity Velocity type On and the second seco			
	O Direction ● Projection ● Magnitude Scale ● Linear ● Logarithmic Scale factor 15.0 ◆ Max. velocity 2.012 Apply QK Car	ncel	Help	

Color

Color options for the velocity vectors apply to the velocities perpendicular to the displayed row, column, and/or layer selected on the <u>General</u> tab. Positive values (default red color

ramp) correspond to the positive X, Y, and Z directions, typically east, north, and up, respectively. Negative values (default blue color ramp) correspond to the negative X, Y, and Z directions, typically west, south, and down, respectively. Areas with velocities below the specified in-plane range threshold will be displayed using the specified In-plane color.

General	Colors					
Style ⊕ - Cells ⊕ - Lines ⊕ - Vertices	Transparency (%)					
	Color					
	In-plane	In-plan	e range			
ThreeSlices IsoSurface	11, 255, 255, 25	5 🗸 2.00	* %			
	Outward start	Outwa	rd end			
VelocityMap	Blue	~ E	lue 🗸		2.012	
Colors	Inward start	Inward	end		2.012	
Legend	Red	F	ed 🗸			
	Color Classification Type	Classes				
		Classes Number	of Classes 9	A V		
	Type		f Classes 9 Value			
	Type Stretched Classified Cc 255, 0, 0	Number	Value 2.011984			
	Type Stretched Classifie	Number	2.011984 1.760486			
	Type Stretched Classified Cc 255, 0, 0	Number	Value 2.011984			
	Type Stretched Classified Cassif	Number	Value 2.011984 1.760486 1.508988 1.25749 1.005992		Î	
	Type Stretched Classified Constitution 255, 0, 0 255, 0 255	Number	Value 2.011984 1.760486 1.508988 1.25749		~	
	Type Stretched Classified Cassified Construction 255, 0, 0 255, 0	Number	Value 2.011984 1.760486 1.509988 1.25749 1.00592 0.7544941			1

Legend

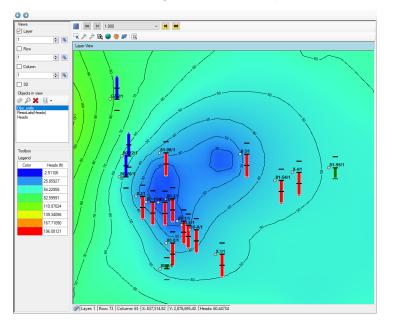
Legend options allow you to format the legend for the velocity colormap.

😂 Settings - Velocity (Nu	mericalGrid_refined-Run/ModelRunResult/3D View)			\times
⊕. General	Legend			
÷ Style ÷ Cells ∵ Lines				
	Legend Properties			
	Legend Header Color			
ie- ThreeSlices ie- IsoSurface ie- Time	Legend Header Font Size 12	×		
· Ime · VelocityMap · General · Colors	Legend Text Color			
Legend	Legend Text Font Size 10	•		
	Number of decimal places 2	-		
	Legend X Position (% of window width) 4	-		
	Legend Y Position (% of window height) 4			
	Apply QK C	ancel	Hel	p

Residuals

(Only available for output residuals)

The ResidualMap settings are only available for output residuals and allow you to visualize the spatial distribution and magnitude of the output observation residuals.



General

Residuals can be displayed by layer/row/column and/or observation group in the specified view:

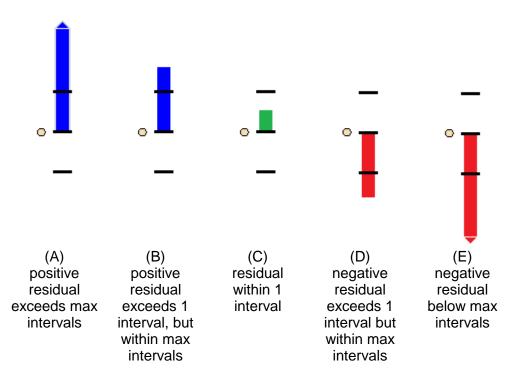
- Visible: if selected, residuals will be displayed using the options described below
- View Points from the following slices: allows you to view residuals that intersect with the selected option:
 - <u>Current Slice</u>: only residuals that intersect the current layer, row, or column (as applicable) will be displayed in the view
 - o All Slices: all residuals will be shown
 - <u>Selected</u>: only residuals that intersect the selected layer(s), row(s), or column(s) (as applicable) will be displayed in the view

💭 Settings - Residuals(H	leads) (NumericalGrid-Run8/I	ModelRunResult/Layer View)			\times
- General	General				
Info Details ⊡- Statistics ⊡- Style ⊡- ResidualMap General	☑ Visible	View points from the following slices: © Current slice All slices Selected slices			
- Residuals - Labels	ayer: 1 ayer: 2 ayer: 3 ayer: 4 ayer: 5 layer: 6				
	Vew points from selected Head Obs 1 Head Obs 2 Head Obs 3 Head Obs 4 Head Obs 5	groups			
		Apply OK C	ancel	Hel	p

Residuals

The Residuals options provide some settings for how the residuals will be displayed on the map:

- Residual Scale: the relative size of the residual symbols shown in the view.
- Max Number of intervals: the number of the target residual intervals beyond which residuals will be truncated. For example, if the target residual for an observation is 0.5 m, and the max number of intervals is set to 3, then an absolute residual value greater than 1.5 m will be truncated, as shown in Case (A) below. Note that truncated values will always be truncated at 2x the target residual regardless of the max number of intervals setting.



- Above target interval: residuals that have a positive value (i.e. the simulated value is greater than the observed value) with a magnitude greater than one target residual interval will be color coded with the selected color (Cases A and B above, default is blue)
- Within target interval: residuals that have a magnitude greater less than or equal to one target residual interval will be color coded with the selected color (Case C above, default is green)
- Below target interval: residuals that have a negative value (i.e. the simulated value is less than the observed value) with a magnitude greater than one target residual interval will be color coded with the selected color (Cases D and E above, default is red)

⊡- General ⊒- Style	Residuals		
	Trostadais		
ia- ResidualMap General Residuals Labels	Residual scale 5.00 Max number of intervals 2 Above target interval		
	Within target interval		
	Below target interval		
	Apply OK	Cancel	Help

Labels

Labels can be optionally displayed next to the Residuals using the following settings:

- Visible: shows/hides residuals labels.
- Well name: includes/excludes the name of the observation point in the label
- Obs values: includes/excludes the observed value at the observation point in the label
- **Calc values**: includes/excludes the simulated value at the observation point in the label
- **Residual values**: includes/excludes the residual value (difference between the simulated value and the observed value) in the label
- **Decimal Places**: sets the number of decimal places that will be used to show the Obs, Calc, and Residual values
- Label Font: sets the font (pt) size
- Label color: sets the color of the label font
- **Show Frame**: shows/hides a frame around the label text and sets the color of the frame
- Show Background: shows/hides a fill color behind the label text and sets the color of the background

Settings - Residuals(I	Heads) (NumericalGrid-Run8/ModelRunResult/Layer View)			\times
Settings - Residuals()	Labels Visible Label details Visible Well name Obs values Calc values Residual values Decimal places			×
	2			
	Apply OK 1	Cancel	Help	2

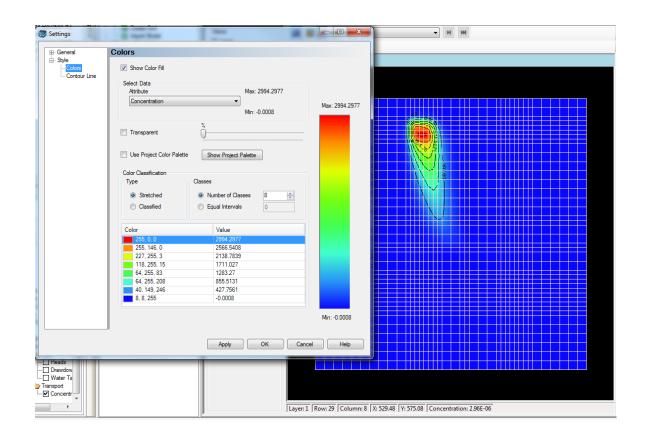
6.3.6 Settings Color Classifications

For those data objects that attributes that can be rendered, you will see a Colors page in the Style node of the Settings page. You can now adjust the values assigned to the colors to suit you needs (for example for Calculated Heads, Concentrations, Kx, etc.). A common application of this would be when you are viewing transport concentrations, and you want a value threshold to be assigned to a specific color (eg. 10 mg/l for a water quality).

Default Color Palette for Transient Data

After a model run, when you first view maps for transient data objects (heads, drawdown, concentration, water table), the color palette you see in the color legend will be a default. The color palette (including min/max values) will be re-calculated each time you change the output time. However, once you load the settings for the specific 2D or 3D view, then the values in the Color Classification will be applied globally for all output times.

Load the settings for the desired 2D or 3D view, and you should see the color page below (this example is for Concentration for the Layer (2D) View).



In the grid at the bottom of the window, you can adjust the value that are assigned the various colors. When using this option, you may wish to set the Color Classification Type to be "Classified". Doing so, will assign a specific color to a range of discrete values. Enter the values working from lowest to highest (from bottom to top).

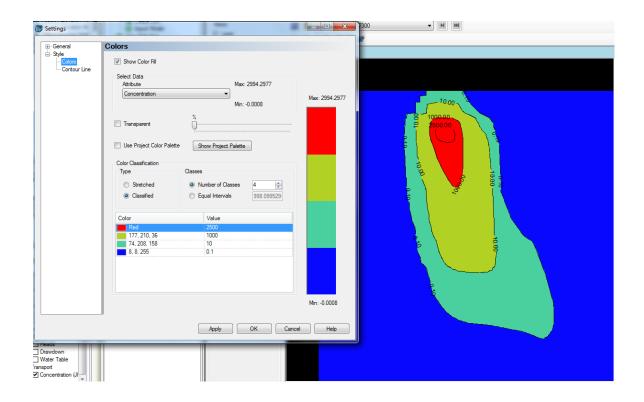
Explanation of Color Values

Using the data set and settings from the figure above, the color values were adjusted as follows.

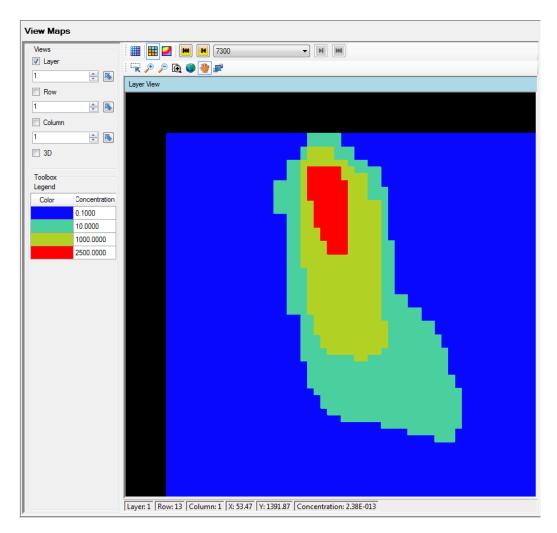
In the example below, there are 4 color classes:

C	olor	Value	Range of Values Assigned to this color
	Red Pale Green Aqua- Blue Dark Blue	1000 10	 >1000 to the Maximum data value >10 to 1000 >0.1 to 10 Minimum data value to 0.1

2D viewer with "Surface" rendering on:



2D viewer with Cells rendering on.



As you change different output times, the user-defined color palette will be honored.

The settings need to be defined separately for the 2D and 3D View. Once you close a view (e.g. stand-alone 3D viewer), the color values will be lost, and you will need to re-define them.

In addition, in the case of rendering for MODFLOW/MT3D results (heads, drawdown, concentrations), the user-defined values will be lost upon re-translating and running the model, so you will need to re-define these values.

6.4 Data Table

The data table allows you to view the data that defines certain objects in the Data Explorer in a tabular format.

• **Shapes** (i.e. Points, Polylines, and Polygons) include tabulated geometry (X-, Y-, and Z-coordinates) and attributes;

- Schedules: include one or more values tabulated for an ordered list of DateTime values as attributes; and
- Wells (observation and pumping wells): include tables defining the locations of wells, screens, pumping schedules and/or observations.

The tables associated with shapes and schedules have a common interface for general tables. Observation and pumping well objects include a more complex interface that links tables for the location of the well borehole (path), well screens, pumping schedule, and/or observations as applicable.

Accessing Data Tables

The data table allows you to view the geometry and attribute values of a data object, including schedule objects and point, polyline, or polygon objects. The data table can be launched by:

- clicking the Table button Table in <u>General</u> settings in the <u>Data Settings</u> dialog, or
- right-clicking on the data object in the Data Explorer, and selecting View Spreadsheet...

Spreadsheet (General Tables)

The **Attribute** tab contains the attribute data of the selected data object. Each column in the attribute tab represents an attribute. The **Geometry** tab contains a list of the vertices (X-, Y-, Z-coordinates) that define the geometry of the data object. In both tabs, the FID column uniquely identifies each feature in the data object. Note that polylines and polygons contain multiple entries in the geometry table for the same FID, since polylines and polygon are made up of multiple vertices.

👺 Spreads	heet							-		🐯 Spr	eadsheet							-	o x
Attribute Geometry							Attribute Geometry												
h 2	80									- 1 Ba	2 🗟 🧿								
FID	< ID	ISEG	IRECH	RCHLEN	STRTOP	STRTOP_DS	SLOPE	STRTHICK	STRH ^	FID	/ ID	ISEG	IRECH	RCHLEN	STRTOP	STRTOP_DS	SLOPE	STRTHICK	STRH ^
• 0	101	1	1	102	2356.5	2352.216	0.042	1	5.787		101	1	1	102	2356.5	2352.216	0.042	1	5.787
1	102	1	2	90	2352.5	2346.74	0.064	1	5.787	1	102	1	2	90	2352.5	2346.74	0.064	1	5.787
2	103	1	3	60	2345.5	2340.52	0.083	1	5.787	2	103	1	3	60	2345.5	2340.52	0.083	1	5.787
3	104	1	4	30	2342.5	2340.07	0.081	1	5.7871	3	104	1	4	30	2342.5	2340.07	0.081	1	5.787
4	105	1	5	102	2336.5	2330.176	0.062	1	5.787	4	105	1	5	102	2336.5	2330.176	0.062	1	5.787
5	106	1	6	90	2332.5	2326.65	0.065	1	5.787	5	106	1	6	90	2332.5	2326.65	0.065	1	5.787
6	107	1	7	90	2324.5	2316.49	0.089	1	5.787	6	107	1	7	90	2324.5	2316.49	0.089	1	5.787
7	108	1	8	90	2316.5	2307.77	0.097	1	5.787	7	108	1	8	90	2316.5	2307.77	0.097	1	5.787
8	109	1	9	102	2306.5	2292.118	0.141	1	5.7871	8	109	1	9	102	2306.5	2292.118	0.141	1	5.787
9	110	1	10	102	2288.5	2269.528	0.186	1	5.787	9	110	1	10	102	2288.5	2269.528	0.186	1	5.787
10	111	1	11	102	2268.5	2246.366	0.217	1	5.787	10	111	1	11	102	2268.5	2246.366	0.217	1	5.787
11	112	1	12	72	2247.5	2232.884	0.203	1	5.787	11	112	1	12	72	2247.5	2232.884	0.203	1	5.787
12	113	1	13	30	2240.5	2234.32	0.206	1	5.787(12	113	1	13	30	2240.5	2234.32	0.206	1	5.787
13	114	1	14	72	2226.5	2211.668	0.206	1	5.787	13	114	1	14	72	2226.5	2211.668	0.206	1	5.7871
14	115	1	15	30	2219.5	2215.18	0.144	1	5.787(14	115	1	15	30	2219.5	2215.18	0.144	1	5.787
15	116	1	16	90	2210.5	2197.27	0.147	1	5.787(15	116	1	16	90	2210.5	2197.27	0.147	1	5.7871
16	117	1	17	102	2196.5	2182.73	0.135	1	5.787	16	117	1	17	102	2196.5	2182.73	0.135	1	5.7871
17	118	1	18	90	2184.5	2172.89	0.129	1	5.7871	17	118	1	18	90	2184.5	2172.89	0.129	1	5.7871
<									>	6									>
					-				-	1					_				
							Apply	ОК	Cancel								Apply	OK	Cancel
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Attribute										G	eom	etrv							

To copy data to the Windows clipboard, highlight the data to be copied, and then click the Copy button and press CTRL+C on your keyboard.



When a data object is shown in 2D Viewer and the viewer is set to Pick Mode, you can select a row from the attribute or geometry table, and the corresponding feature will be highlighted in the 2D Viewer.

Modifying Attribute and Geometry Data

Geometry and attribute data can be modified in the Data Table. To make changes to data, click the Begin Edit button to enter edit mode. Make the necessary changes to the data table and once finished, click the End Edit button to save the changes. Please note that the data table only allows you to modify existing attribute and geometry data. Currently, Visual MODFLOW Flex does not allow you to create new columns (i.e., new data object attributes) or rows (i.e. new geometric features). New attribute fields can only be done during the data import process. However, you can adding geometric features during an <u>edit session</u> in a 2D view.

Well Table

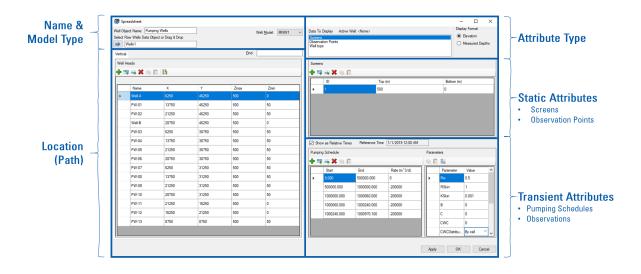
For Wells data objects, the data table is different than that of other data objects. The Well data table is designed to allow you to add and/or modify wells and associated well data, e.g., well locations, pumping schedule, screen intervals, observation points, etc. The data tables for wells are defined in the <u>Well Data</u> section.

6.4.1 Well Data

This section describes the data view for well objects that may contain any of the following information:

- Location
- Borehole path (for non-vertical wells only)
- Screen location(s) and characteristics
- Observation points
- Pumping schedule
- · Observed heads and/or concentrations

In the Well Table, this information is divided into separate panes that store information about the well options, location, static attributes, and transient attributes.



Apart from some subtle differences discussed below, the Well Table dialog is the same whether the well set is:

Data Explorer

• Well object

Model Explorer

- Pumping Wells in a Conceptual Model
- Pumping Wells in a Finite Difference Model

Note that wells are currently handled as simple non-conceptual boundary conditions in unstructured grids.

Name

The well data pane includes an option to add a name for the Well Object. This name is the label that is shown in the Data Explorer for well objects and in the Model Explorer for the Conceptual or Numerical Model, as applicable. The name of the well can be edited and if applied or accepted, the edited well name will be displayed in the Data Explorer or in the Model Explorer as applicable.

Well Model Type

The data that defines how a set of pumping wells is represented in the groundwater model is based on the Well Model selection. Available well models are based on the boundary condition package that will be used to represent wells in the numerical model. Visual MODFLOW Flex supports WEL, MNW1, and MNW2 packages. See the <u>Theory</u> section for a description of each model.

Well Location/Path

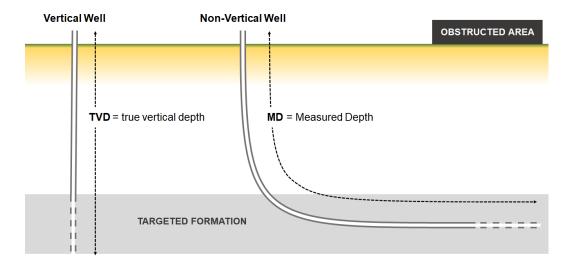
The Well Heads table contains a list of all the wells in the data object. The data stored in this table includes the Name, X-Y coordinates, Elevation and Depth for each well. When a well is selected, its corresponding attribute data is displayed in the adjacent data tables, e.g., Screens, Pumping Schedule. You can search for a well in the Well Heads table by entering the well name in the text box, located at the top of the window, and then clicking the [Find] button.

Vertical Wells vs. Non Vertical Wells

Most commonly, wells are constructed within the shaft of a vertical borehole. Such vertical wells are most efficiently defined by a constant horizontal position (X/Y co-ordinates) and a list of true vertical depths or elevations (z co-ordinates) to denote the top and bottom of the well and its screen(s). In the case where the well is defined using a true vertical depth, a reference elevation must also be provided.

However, there are many situations where a vertical well may not be feasible (e.g. limited/restricted access to the target formation at ground level due to property access or existing infrastructure at or near ground surface) or desirable (e.g. one or more vertical wells do not provide sufficient/cost-effective hydraulic connection to the target formation). In such cases, non-vertical wells (sometimes called horizontal or directional wells) may be used.

Depth along Non-vertical wells is non-trivial and requires a more complex data structure that includes a list of X-Y-Z vertices sufficient to describe the entire path of the well. The list of such vertices is called the Well Path. Since the well path may include horizontal or even ascending sections along its "depth", features along the well must be described in terms of the measured depth (i.e. the length along the well path as measured from the well head).



If the wells in the Well object are vertical wells, the Vertical tab containing the Well Heads table will be displayed. If the wells in the Well object are non-vertical wells, the Non-Vertical tab containing both the Well Heads table and the Well Path table will be displayed.

Converting Vertical Wells to Non-Vertical Wells

You can convert vertical wells to non-vertical (i.e. horizontal/directional wells) by pressing the button; however, note that the conversion from vertical wells to non-vertical wells is a one-way process.

Well Heads Data

The Well Head table will be displayed for both vertical and non-vertical wells. The well heads table allows you to view the location and general information of each well in the well set, including the name of the Well, the X and Y coordinates and well top and bottom. Note that the well bottom will not be displayed for non-vertical wells, since the well bottom will be described by the final vertex in the well path.

Interview Well: <none> Display Format</none>
Top (m) Bottom (m)
Top (m) Bottom (m)
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ê f i
End Rate (m^3/d)
3650.000 -29.6

Adding Well Head Data

To add an item to the Well Head table, follow the steps below:

- Click the Add Row button from the Well Head toolbar to add a new item to the table.
- Enter an alphanumeric name in the Well Name column. Note: The well name must be unique and it may contain hyphens and spaces, but not the forward or backward slash characters.
- Enter the X-Y coordinates of the well head in the X and Y fields, respectively.
- Enter the elevation of the well head in the Zmax field.
- Enter the depth of the well in the Zmin field.

Non-Vertical Wells

The Well Path tab includes a table for the selected well with the following field headings:

- ID: the index of the vertex
- X: the x-coordinate of the well path for the ith point
- Y: the y-coordinate of the well path for the ith point
- Z: the Z-coordinate of the well path for the ith point

Obje	ect Name: Non-Ver	tical		Well Model: M	INW1 V	Data To Display Activ Screens Observation Points Well tops	e Well: <none></none>				splay Format Bevation Measured Dept
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Attribute Types

The Data to Display list box allows you to select which well information tables to display. For example, if Screens is selected (default), the <u>Screens</u> information (Screens and Pumping Schedule tables) will be shown. If Observations is selected, the <u>Observation</u> information (Observation Points and Observation Data tables are shown. If Well Tops is selected, the <u>Well Tops</u> table will be shown.

The Display Format frame allows you express the Z values in the data tables as either an Elevation or a Measured Depth (with respect to the well head Zmax).

At the top of each table, there is a set of buttons that allow you to add, remove and modify the contents. The function of these buttons, in order from left to right, is described below:

- Add a row to the table
- Insert a row above the active row
- Insert a row below the active row
- Remove the active row from the table

Screens

The Screens attribute table contains the Well Screen table and the Pumping Schedule as described below:

Well Screens

The Well Screens table includes the following field headings:

- ID: a unique name for the well screen
- Top (Elevation/Depth): the top of the well screen
- Bottom (Elevation/Depth): the bottom of the well screen

Please Note: in non-vertical wells, the screen tops/bottoms can only be defined using the measured depth (see discussion <u>above</u>)

Adding a Well Screen

To add an item to the Well Screen table, follow the steps below:

- Make sure the Screens option is selected from the Data to Display box.
- Select a Well from the Well Head table
- Click the Add Row button from the Screens toolbar to add a new item to the table.
- Enter a screen identification number in the Screen ID field.
- Enter a screen top elevation (or measured depth) in the Screen Top field.
- Enter a screen bottom elevation (or measured depth) in the Screen Bottom field.

Pumping Schedule

Adding/Editing Pumping Well Schedule

The Pumping Schedule table is used to enter the well pumping rates for specified time periods. Negative pumping rate values are used for extraction wells, and positive pumping rates are used for injection wells.

Pumping well schedules are defined for the entire well, and therefore a screen must exist before a pumping schedule can be defined.

To add pumping schedule items to the pumping schedule table:

- Make sure the Screens option is selected from the Data to Display box.
- Select a Well from the Well Head table, and a Screen from the Screen Table (if multiple screens exist)
- Click the Add Row button from the Pumping Schedule toolbar to add a new item to the table.
- Enter a Start time value and press the <Tab> key to advance to the End time field.
- Enter an End time value and press the <Tab> key to advance to the Rate field.
- Enter a pumping Rate value (remember to use a negative value for extraction wells)
- Press the <Tab> key again to create a new schedule item.

• The final time in the pumping schedule should have a pumping rate of 0 to indicate the stop time.

Please Note: If the pumping schedule is not specified for the entire length of the transient simulation, then Visual MODFLOW Flex will assume the well is shut off for the time where no information is available at translation. For steady-state simulation, the pumping rate for the first time period will be used as the steady-state pumping rate.

When selected, the "Show as Relative Times" checkbox will display time schedule data starting at 0, and times will be displayed relative to the start date defined in the Modeling Objectives; this is useful when you want to correlate the raw well data to MODFLOW time formats. When this option is not selected, then time schedule data will appear in "Absolute" (calendar) time formats.

Observations

Observation Points

Observation Points are the elevations at which head or concentration observations are recorded. Although most monitoring or observation wells are installed with a well screen spanning a known interval of the aquifer, Visual MODFLOW Flex requires a single observation point elevation to be defined instead of a well screen interval.

Adding Observation Points

To add an observation point for a well:

- Select the Observations option from the Data to Display box. This will show the Observation Points table.
- Select a well from the Well Heads table
- Click the Add Row button from the Observation Points toolbar to add a new item to the table.
- Enter an observation point ID in the ID field.
- Enter an elevation value in the Elevation field.

The MODFLOW simulator supports head and concentration observation wells with multiple observation points throughout the length of the well-bore. Repeat the steps above to add additional points.

Observation Data

Adding Head Observation Data

The Observation Data table is used to enter the observed values at specified times, for the selected observation point.

To add observations to the Observation Data table, follow the steps below:

- Select Observations from the Data to Display box.
- Select the well from the Well Heads table for which observation data will be added.
- Select the desired observation point from the Observation Points table.
- Click the Add Row button from the Observation Data toolbar to add a new item to the table.
- Enter the time at which the head was observed in the Time field.
- Enter the observed head values in the Head field.

The "Show as Relative Times", when selected will display time related data starting at 0, and relative to the start date defined in the Modeling Objectives; this is useful when you want to correlates the raw well data to MODFLOW output time. When this option is not selected, then time related data will appear in "Absolute" (calendar) time formats.

Adding Concentration Observation Data

If you imported well data with <u>concentration observations</u>, the observation data tab will include concentration observations. The table will include same information as the heads observation data except that there will be a species field to identify which transport species was observed and the observed values will have units of concentration (M/L³) instead of head (L). Note the name of the species must EXACTLY match the Name of the Species in the Modeling Objectives for it to be tied to the modeling output residuals and charts.

Well Tops

The Well tops table is used to enter the elevation points along the well path, where the well intersects with a horizon. Well top information can be used in Visual MODFLOW Flex to create surfaces which can then be used to define conceptual model horizons. For more information on creating surfaces from well tops, please see "<u>Converting Well Tops to Points</u> <u>Data Object</u>" section.

To add well top information to the Well Top table, follow the steps below:

- Select Well Tops from the Data to Display box.
- Select the well from the Well Heads table for which well top data will be added.
- Click the Add Row button from the Well Tops toolbar to add a new item to the table.
- Enter the location of the well top as a measured depth in the Depth field.
- Enter the name of the formation, e.g., Clay, Sand etc., in the Formation field.

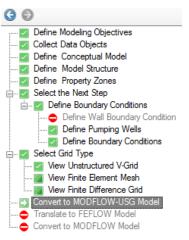
7 Conceptual Modeling Workflow

A Conceptual Model refers to a high-level representation of the hydrogeologic system being modeled. It will form the foundation for one or more numerical models. In Visual MODFLOW Flex, the conceptual model is completely grid- and simulator-independent. This means, you define the inputs using your raw data objects (surfaces, polylines, polygons, etc.). The grid or mesh is only introduced at the time of launching a numerical model. This allows you to:

- Convert the conceptual model to multiple grids and/or numerical models for different analyses through the modeling process:
 - o coarse models for fast runs
 - o refined models with greater detail/resolution
 - o scenario analysis
 - o uncertainty analysis
- Easily update corresponding numerical models as your conceptualization changes

The sequential steps in building the conceptual model are presented in the workflow navigator and are summarized below:

- 1. Define Modeling Objectives
- 2. <u>Collect Data Objects</u> (through importing or creating)
- 3. Define the Conceptual Model Area
- <u>Define Model Structure</u> (vertical layering and resulting volume models)
- 5. <u>Define Property Zones</u> (parameter values for Conductivity, Initial Heads, Storativity)
- 6. <u>Define Boundary Conditions</u> (constant heads, drains, pumping wells, surface water network, etc)
- Select Grid Type: (Define Finite Difference Grid, Define Finite Element Mesh, or Define UnStructured Grid)
- 8. <u>Convert to Numerical Model</u> (generate numerical inputs for a MODFLOW model)
- 9. <u>Translate to Finite Element Model</u> (generate FEFLOW ASCII .FEM file for running in FEFLOW)



10 Convert to MODFLOW-USG Model

(generate numerical inputs for a MODFLOW USG model)

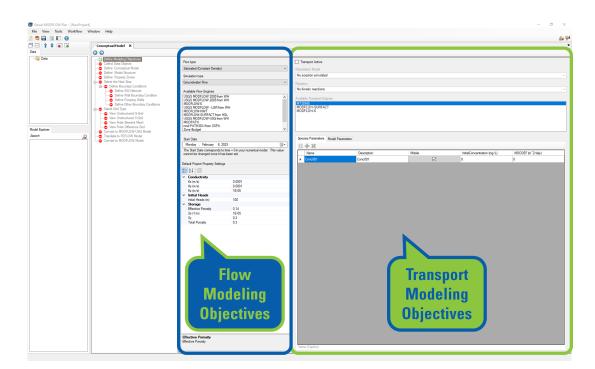
When a new conceptual model is created, a new Model Explorer tree is added to the Conceptual Model Explorer in the main Visual MODFLOW Flex window.

The Model Explorer tree consists of a fixed folder structure that is designed to guide you through the workflow of building your conceptual model.

7.1 Define Modeling Objectives

The first step in defining your conceptual model is to Define the Modeling Objectives, as shown below. Modeling Objectives are divided into two sections:

- Flow Objectives
- Transport Objectives



Visual MODFLOW Flex supports numerous groundwater flow modeling codes (or generalized models) developed by the USGS and others. For the purposes of clarity and to distinguish these generalized models from particular regional and site-specific models that are developed to run with them, these modeling codes are referred to as "engines" within the Visual MODFLOW Flex interface. Each engine was developed to support simulations of

groundwater systems with a certain set of conditions, processes, and underlying assumptions, some of which are common to all engines and some of which may only be applicable to one or a subset of engines. Visual MODFLOW Flex currently supports the following engines to facilitate simulations of groundwater systems under a wide variety of conditions:

Flow Engine	Compatible Transport Engine	Compatible Utilities
 MODFLOW-2000 MODFLOW-2005 MODFLOW-NWT 	MT3DMSRT3D	 ZONEBUDGET MODPATH MOD-PATH3DU⁵ PEST
MODFLOW-LGR		
• MODFLOW-USG ¹		 ZONEBUDGET- USG MOD-PATH3DU⁵
MODFLOW-6 ²	MODFLOW-6 ²	• ZONEBUDGET-6
 MODFLOW- SURFACT³ 	 MODFLOW- SURFACT³ 	MODPATH
• SEAWAT ⁴	 SEAWAT⁴ 	ZONEBUDGETMODPATH

Engines supported in Visual MODFLOW Flex

Notes:

1 - MODFLOW-USG uses unstructured grids and is supported under a <u>separate workflow</u> process as compared to the standard <u>numerical workflow</u>.

2 - MODFLOW-6 may be configured to run flow and transport simulations in series or within a single coupled simulation.

3 - MODFLOW-SURFACT is a commercial groundwater modeling engine that supports coupled groundwater flow and transport simulations. A demo version of MODFLOW-SURFACT is included with Visual MODFLOW Flex; the full commercial version is sold separately.

4 - SEAWAT is a coupled variable density groundwater flow and transport model

5 - MOD-PATH3DU is a particle-tracking algorithm developed by a collaboration between S.S. Papadopulos & Associates (SSPA) and the University of Waterloo. It is not installed directly with Visual MODFLOW Flex and must be downloaded and installed separately from the <u>mod-PATH3DU</u> website.

Flow Objectives

The first step in the workflow for developing and running numerical models in Visual MODFLOW Flex is to define the modeling objectives. This entails selecting the desired flow and transport simulation options. The selected combination of flow options (e.g. saturated groundwater flow) and transport options (e.g. reaction and sorption models) will narrow the list of available flow and transport engines and generate associated input variables (including units and default values). The purpose of this step is to develop the necessary inputs required to build the model based on your understanding of the relevant physical processes present within the study area.

The flow engines supported in Visual MODFLOW Flex are presented in the table below, which provides a preview of what engines are available based on your selected flow and simulation types.

Flow Type		Туре	Fle	rated ow		/ariably	/ Satur	ated Fl	ow ¹			ticle king	
Simulatio n	ured	ucture		Variab le	Gro	bundwa	ater	Vapo	or Flow	Zone Budge	MODP	MOD- PATH	
Туре	Grids	d Grids	Densit y	Densit y	UZF	V	BC	V	BC	t	ATH	3DU	port
Engine	S							-	-	-			
MF- 2000										V	\checkmark	$\mathbf{\nabla}$	
MF- 2005					\checkmark					V			V
MF-6 ²										ZoneB udget- 6			MF-6
MF- NWT					\checkmark					V			V
MF- LGR													
MF- USG²		V								ZoneB udget- USG			
SEAW AT	V									V			SEAW AT
MF- SURFA CT	V						V	V	V			V	MF- SURF ACT

Flow Engines, Grid Types, and Modeling Objectives Supported in Visual MODFLOW Flex

Notes:

1 - Abbreviations for variably saturated flow processes in the Vadose Zone:

UZF = unsaturated zone flow package is based on 1-D unsaturated flow of a diffusion wave pseudo soil V = Van Genuchten relative permeability and saturation relationship

BC = Brooks-Corey relative permeability and saturation relationship

2 - MODFLOW-6 and MODFLOW-USG support more modeling objectives than currently available in Visual MODFLOW Flex, these will be added in subsequent releases. In order to help us better prioritize these, please reach out to our support team (<u>support@waterloohydrogeologic.com</u>) to let us know which objectives you'd like added.

Under Property Settings, you can modify the default flow parameters.

MODFLOW-LGR & MODFLOW-USG and Transport

The MODFLOW-LGR and MODFLOW-USG flow engines do not currently support solute transport.

Setting the Start Date

The **Start Date** of the model corresponds to the beginning of the simulation time period. It is important to define a relevant start date since your field measurements (observed heads and pumping schedules) will be defined with absolute (calendar) date measurements, and must lie within the simulation time period.

Start Date
The start date will be used to retrieve pumping well and head/concentration observation data for the model run. When you define well data with absolute (calendar) dates, it is important that your start date reflects the actual start time for the model run. Absolute time well data must fall on or after that start date . Otherwise, these data will not be included in the simulation.
Also the start date cannot be changed once it has been set. If you inadvertently set the wrong start date, you can import your pumping well data and observation data in relative times (e.g. starting at 0), and you will see no difference in the numerical model inputs/outputs.

Visual MODFLOW Flex uses a standard Windows date picker; a few tips are shown below on how to use this. By default, the current date will be set as the Start Date but you are encouraged to set this to an appropriate date for your model simulation.

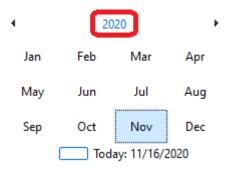
Click on the button shown below, to load the Windows date picker.

🐯 Visual MODFLOW Flex - [Exercise]						- 0 ×
File View Tools Workflow	Window Help					
2 😋 🔚 🔢 🗈 🖓						
	Conceptual Model x					•
Data	GO					
	Control Define Modeling Degetities Context Data Objects Define Conceptual Model Define Property Zones Select the Next Step Define Boundary Conditions Define Pumping Wells Define Deming Wells Define Pumping Define Pumping Wells Define Pumping Wells Define Pumping Wells Define Pumping Define Pumping	Row type Saturated (Constant Density) Simulation type Groundwater Row Available Row Engines USSS MODE/OW 2000 from WH USSS MODE/OW 2000 from WH USSS MODE/OW-LOR from WH MODE/OW-SUFFACT from HSL	Transport Active Retardation Model No sorption simulated Reaction No kinetic reactions Available Transport Engines THEOMS MODFLOW-SURFACT			v
Model Explorer Search &	Vew Finte Bernert Mesh Vew Finte Difference Grid Convert to MODFLOW-USG Model Translate to FEFLOW Model Convert to MODFLOW Model	ZONEBUDGET MODPATH Start Date Tureday , July 11, 2017 ••• The Start Date corresponds to time = 0 in your numerical model. This value cannot be changed more than been eart	Species Parameters Mode	el Parameters Description	Mobile	InitialConcentration (mg/L)
		Changed office it mas been det. Default Project Vpenty Settings QL Kc (m/n) Mark Project Vpenty Settings V Initial Heads (m) No Xorage Storage Storage Storage Initial Heads (m) Initial Heads (m) Initial Heads (m) Initial Heads (m) Initial Heads (m)	Carcoll Carcoll Name (Caption)	Conc.001		0

The standard Windows calendar will appear. Click on the month in the header (as shown below):

4	- (Nove	ember	2020		►
Sun	Mon	Tue	Wed	Thu	Fri	Sat
25	26	27	28	29	30	31
1	2	3	4	5	6	7
8	9	10	11	12	13	14
15	16	17	18	19	20	21
22	23	24	25	26	27	28
29	30	1	2	3	4	5
		T	foday:	11/16/	2020	

All months for the current year will appear as shown below. Click on the year in the header:



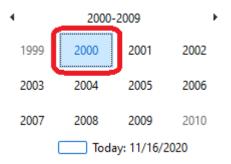
A range of years will then appear as shown below. Click on the range of years in the header:

4	2000-2099							
1990-	2000-	2010-	2020-					
1999	2009	2019	2029					
2030-	2040-	2050-	2060-					
2039	2049	2059	2069					
2070-	2080-	2090-	2100-					
2079	2089	2099	2109					
Today: 11/16/2020								

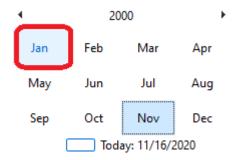
A list of years for the previous decade will appear.

You can then use the < or > buttons to change the year.

Once you have reached the desired year (2000 for this example), select this on the calendar as shown below:



A list of months will then appear for that year. Select January for this example, as shown below.



Finally, select "1" from the calendar as shown below:

4	January 2000				►	
Sun	Mon	Tue	Wed	Thu	Fri	Sat
26	27	28	29	30	31	1
2	3	4	5	6	7	8
9	10	11	12	13	14	15
16	17	18	19	20	21	22
23	24	25	26	27	28	29
30	31	1	2	3	4	5
Today: 11/16/2020						

The selected date will then appear for the Start Date.

Transport Objectives

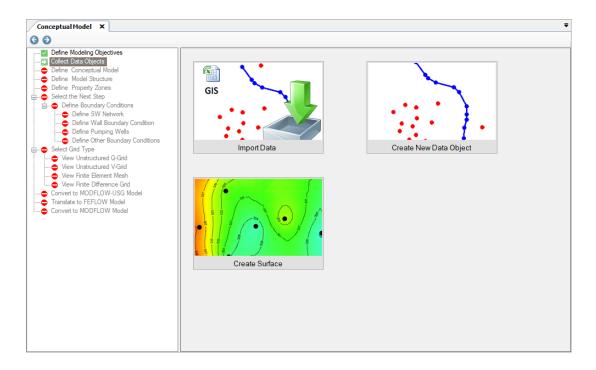
An explanation of the Transport Objectives is available in the section <u>Numerical Model -</u> <u>Define Objectives</u>

Contaminant transport simulation can be enabled and setup in the conceptual model workflow. The species concentrations (for sinks/sources) can be defined while you define your conceptual boundary conditions. However, the transport properties (initial concentrations, dispersion, etc.), are defined in the Numerical Model workflow, after you have defined a grid, and completed the "Convert to Numerical Model" step. This is explained in the section <u>Define Properties (Numerical Model</u>)

• Click 🕑 (Next Step) to proceed.

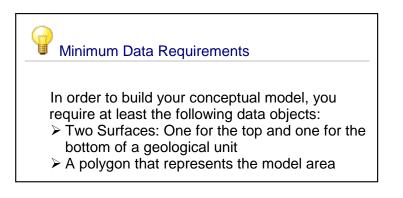
7.2 Collect Data Objects

At this step in the workflow, you collect the data you want to use to build and interpret your conceptual model:



The conceptual modeling workflow is data driven. This means that you first need to "collect" the appropriate data objects in order to use these at a particular step in the workflow. Data objects can be "collected" through several means:

- Importing Data : Import GIS data (shapefiles, CAD files), Gridded data, images, points/wells in excel spreadsheets, or XYZ points in text format.
- > Creating Data Objects: digitizing new point, polygon, or polyline data objects.
- Creating Surfaces: Interpolate XYZ points using Kriging, Natural Neighbor, or Inverse Distance. The resulting surfaces can be used to define geological layers or 2D parameter distributions (Kx, Recharge, etc.)



Once you have the data loaded, Click 🕑 (Next Step) to proceed.

You may return to this step in the workflow at any time during the model process to import or create new data objects.

See the following table for some typical data object types and how they are used in the conceptual model workflow.

If you have	First you should	Then you can
River locations in a shapefile	Import these as Polyline data objects	Select this data object when creating a river boundary condition
Geological layers in a Surfer .GRD or ASCII GRD	Import these as <u>Surface</u> data objects	Select these data objects when defining horizons
Air photo with river location	Import this as a <u>Map</u> <u>image</u> Then <u>Create a new</u> <u>Polyline</u> data object Digitize the polyline in a 2D Viewer	Select this new polyline data object when creating a river boundary condition
XYZ points for geological contacts	Import these as <u>Points</u> data objects Then "Create Surfaces" from these data objects	Select these surfaces when defining horizons or numerical model layers
Raster Grid of Kx or Recharge data (from Surfer, ESRI .GRD)	Import these as surface data objects	Select these data objects when defining properties or Recharge boundary conditions

7.3 Create New Conceptual Model

At this step, provide a name for the model and a conceptual model area as defined by a polygon from the Data Explorer.

3	Visual MODFLOW Flex	x - [usg-transient] – 🗖 🗙
File View Tools Workflow Image: Second	Vindow Help Conceptual Model 2 × Unstructured G Conceptual Model 2 × Unstructured G Conceptual Model 2 × Unstructured G Collect Data Objects Define Model Structure Define Property Zones Select the Next Step Define Boundary Conditions Define Wall Boundary Conditions Define Wall Boundary Conditions Select Grid Type Define Boundary Conditions Select Grid Type View Unstructured V-Grid Wew Finite Elfference Grid View Finite Elfference Grid Convert to MODFLOW Model Convert to MODFLOW Model	irid1-Run1 X Save Name* Conceptual Model 2 Description Model Area Select existing data object Polygon1 Projection Type Coordinate Systems:* Local Cartesian Datum:* World Geodetic System 1984

Quick Overview

Instructions:	Provide a name and a polygon for the conceptual model area
Pre-requisites:	A polygon data object has been <u>imported</u> or <u>created</u>
Result:	Model Explorer tree is defined with the Model Boundary
Next Steps:	Define Model Structure

Once you have imported sufficient raw data into your project, you can begin to construct one or more conceptual models using imported or digitized data objects as building blocks. At this step, you need to define some basic information about the conceptual model, and provide a polygon that represents the model area.

You can import a polygon shapefile/DXF file, as described in the section Import Polygons

Or, if you do not have a polygon, you can create an empty polygon data object, then digitize the geometry. Please refer to the section <u>Creating New Data Objects</u> for more details.

In the Define Conceptual Model window (as shown above), define the settings for the conceptual model.

• Enter a unique name for the conceptual model in the Name field.

- Enter a description of the conceptual model in the Description field (optional).
- Specify a start date from the Start Date combo box. This will be used for calculating the start date for transient model runs.

Please Note: If you are using pumping wells, the start date must match the first start time for your pumping schedule.

• From the Data Explorer, select the polygon data object that represents the conceptual model horizontal boundary, and then click the button.

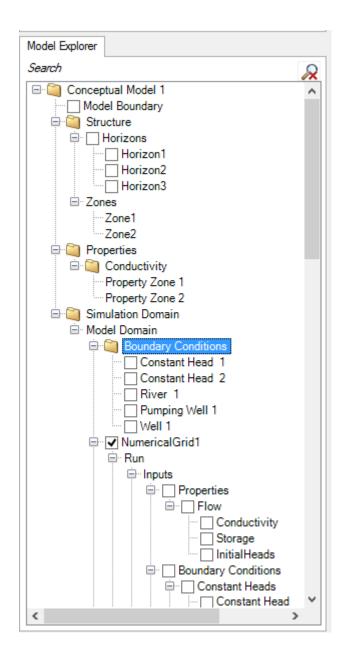
Please Note: The model area must be defined using a simple polygon. It cannot be defined using a complex polygon or one that contains multiple polygons. A complex polygon is a polygon that intersects with itself and/or contains holes.

• Click the [Save] button.

Once you are finished, click 🕑 (Next Step) to proceed.

Model Explorer Tree

Once a conceptual model is created, a new Conceptual Model tree is added to the Model Explorer. The conceptual model tree sets up the workflow for structural and property modeling, assigning boundary conditions, numerical grid creation, and numerical model translation. A typical conceptual model tree is shown below:



The Model Boundary node allows you to show/hide the conceptual model boundary in a 2D or 3D Viewer.

The Structure folder allows you to define the horizons and structural zones of the conceptual model. For more information on structural modeling, please see "<u>Defining the Structure</u>".

The Properties node allows you to define property zones for the conceptual model. For more information on property modeling, please see "<u>Defining Property Zones</u>".

7.4 Defining the Structure

452

At this step, provide the geological surfaces that will represents the tops and bottoms of the geological model.

Visual MODFLOW Flex - [Example] - [Conceptual Model]			
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Grund Grund	Define Conceptual Model Structure		
Convert to MODFLOW Model	Surfaces	Name	Туре
Model Explorer			
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– 🔁 Properties – 🔁 Simulation Domain			
			4

Quick Overview

Instructions:	s: Define geological surfaces for your conceptual model and provide Horizon hierarchy rules	
Pre-requisites:	Two or more surface data objects have been created or imported.	
	created of imported.	
Result:	Horizons and Structural Zones are created	
Next Steps:	Define Property Zones	

At this step, you define the geological structure for the conceptual model, by converting surfaces to Horizons.

Horizons are stratigraphic layers (2D surfaces with topography) that define the upper and lower boundaries of the structural zones in a conceptual model. In Visual MODFLOW Flex, horizons are created by clipping or extending interpolated surface data objects to the boundary of the conceptual model.

When horizons are created, Visual MODFLOW Flex will automatically generate the Structural Zones (geologic formations) between the horizons, which can be used later to define property zones.

This segment is separated into the following sections:

- Defining Horizons
- Explanation of Horizon Types
- <u>View Structural Zones</u>

Defining Horizons

Before You Start!	
objects that you w geological model. imported as expla <u>Objects</u> step. Also, it is currently	ave all the surface data vant to use to construct the Surfaces can be created or ined at the <u>Collect Data</u> y not possible to change the model structure has been

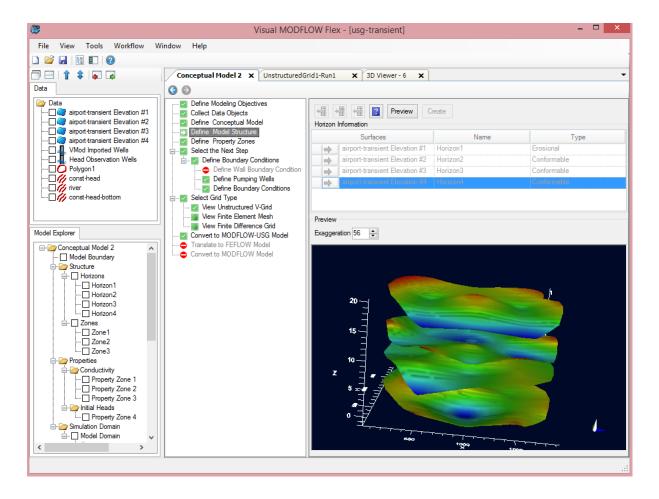
To create a new horizon:

- From the Data Explorer, select the surface data object that will be used to generate the horizon.
- Click the Blue Arrow button to insert it into the Horizon Information table. If the selected surface is greater than the conceptual model area, it will be clipped by the conceptual model boundary polygon. If the surface is less than the conceptual model area, it will be extended to the conceptual model boundary.

Please Note: Surfaces should be added from top to bottom, starting with the top surface (ground surface) and ending with the bottommost surface.

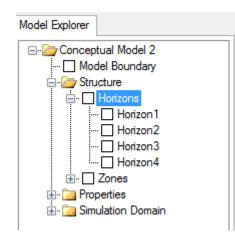
- Click the Add Horizon button to add a new horizon row to the Horizon Information table.
- In the Name column, type in a unique name for the horizon.

- In the Type column, select the appropriate horizon type from the combo box. For information on each horizon type, please refer to "<u>Horizon Types</u>".
- Repeat the steps above to add additional horizons. Remember you must have at least two horizons before Visual MODFLOW Flex can create the structural zones.
- You can preview the horizons in 3D Viewer, by clicking the [Apply] button.



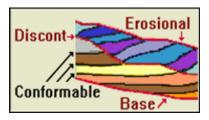
• Finally, click the [] button to create the horizons and proceed to the next step.

Once created, the horizons will be added to the Model Explorer Tree under the Horizons node (shown below).



Horizon Types

Each horizon can be assigned a particular type, which defines the relationship to other horizons in the conceptual model. This prevents intersecting layers and establishes layers that satisfy both FEFLOW and MODFLOW requirements. Each horizon type is described below.



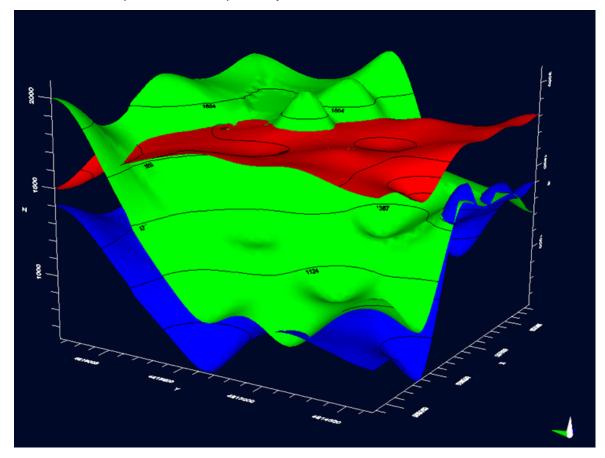
- **Erosional horizons** can be used as the highest or as an intermediate horizon, but not as the bottom of the conceptual model. This type of horizon will truncate all horizons below it, including the base horizon.
- **Base horizons** can be used as the lowest horizon in the conceptual model. Any conformable horizon types will lap onto it, while all erosional or discontinuity horizons will truncate it.
- **Discontinuity horizons** represent an erosional surface in the middle of a stack of horizons. It can never be the highest or lowest horizon. Horizons above it up to the next discontinuity or erosional horizon will lap onto it, while all horizons below it will be truncated by it. These horizons can be thought of as the top or base of a sequence.
- **Conformable (default) horizons** will be truncated by erosional, base and discontinuous horizons. Lower conformable horizons will be truncated by upper conformable horizons. If a conformable horizon is above an erosional horizon, the conformable horizon will "conform" to the erosional horizon (it will be pushed up by the erosional horizon).

The horizon rules described above are applied after all the horizons are calculated. If one of the horizons will be truncated by an erosional, base, or discontinuity horizon, it is a good idea

to extend the input data beyond these unconformable horizons in order to truncate them properly.

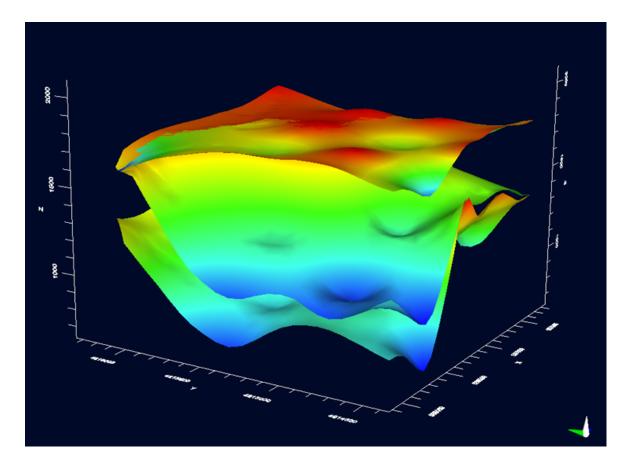
Demonstration of Horizon Types

The image below shows three surfaces in a 3D Viewer. The surfaces are colored Red, Green, Blue, from top to bottom, respectively.

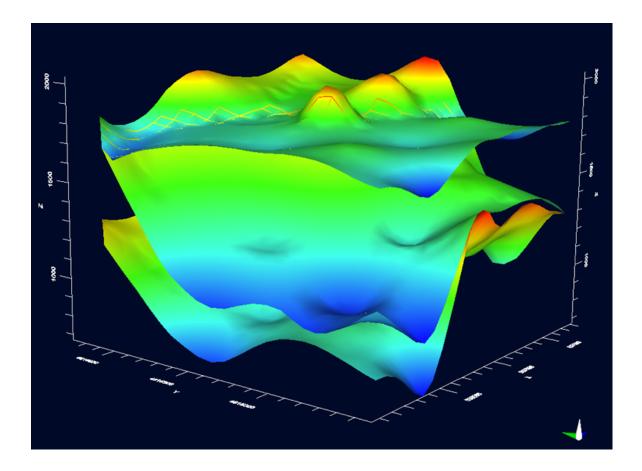


You will see that there are spots where the green surface intersects with the red surfaces, and likewise, where the blue surface intersects with the green surface. For numerical models, this geometry is not permitted (as it will lead to zones with negative thickness), which is why surfaces are converted to horizons. Assigning a horizon type will eliminate the intersections.

When horizons are generated from these surfaces, and each surface is set to Conformable by default. Conformable horizons are truncated such that each one conforms to the horizon above it, as shown in the following image.

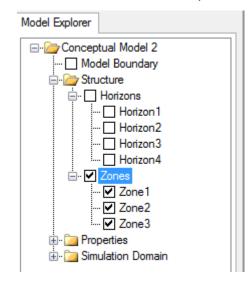


If the middle horizon is set to Erosional, with the top and bottom set to Conformable, the topmost surface (red) is pushed up, as shown in the following image.



View Structural Zones

During the horizon creation process, Visual MODFLOW Flex automatically generates the structural zones between the defined horizons within the horizontal extent of the conceptual model boundary. To view the generated structural zones, in the Model Explorer Tree, expand the Structure Node and then expand the Zones node.



Structural Zones are given a default name, e.g., Zone1, Zone2, Zone3 etc., which cannot be modified.

You can view the zones in an active 3D Viewer window by checking the empty check box beside the zone name. For more information on data viewers, please refer to "Data Viewers" section.

7.5 Defining Property Zones

At this step of the Conceptual Modeling Workflow, you can define the flow property values for the geological formations.

(3)	Visual I	MODFLOW Flex - [Conceptual Modeling	g Tutorial]		- 🗆 🗡
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	Conceptual Model 1 ×				*
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	Conceptual Model 1 X Conceptual Model 1 X Conceptual Model 2 Opticities Conceptual Model 2 Optice Model 2 Optice Model 3 Optice 2 Optice 3	Ceate New Property Zone Method Use Structural Zone(s) Use Polypon Data Object Name Description	Select one or more structural zones	Property Zones	
	< >>				

Quick Overview

- Instructions: Define flow properties for the conceptual model
- Pre-requisites: <u>Structural Zones are created.</u>
 - If you wish to use a spatially-distributed property values, you have imported or created surfaces.

	 If you wish to subdivide zones into lateral regions, you have imported polygon shapefile(s) or digitized polygons.
Result:	One or more property zones are created
Next Steps:	Define Boundary Conditions

At this step, you define Property Zones for the conceptual model. Each property zone is assigned appropriate property attributes, e.g., conductivity, storage, and initial heads.

A groundwater flow model requires many different types of data to simulate the hydrogeologic processes influencing the flow of groundwater. In Visual MODFLOW Flex, the hydrogeologic characteristics of the model are classified into the following parameter groups for flow models:

- **Conductivity**: horizontal conductivity in the horizontal/x-direction (Kx), in the horizontal/y-direction (Ky) and in the vertical/z-direction (Kz)
- **Storage**: specific storage (Ss), specific yield (Sy), effective porosity (Ep), total porosity (Tp)
- Initial Heads: starting head values in the model

By default, Visual MODFLOW Flex automatically assigns the default property parameter values, specified in the Project Settings (see "Project Settings" for more details) to the entire model domain. However, in most situations, the flow properties will not be uniform throughout the entire model domain, and it will be necessary to assign different property values to different areas of the conceptual model. This can be accomplished by creating Property Zones. In Visual MODFLOW Flex, a property zone is a specified 3D-volume, generated from structural zones, with user-defined hydrogeologic attributes.

Property zone geometry can be defined using one or more existing structural zones. As such, property zones can only be generated after horizons have been defined in the conceptual model. Please see <u>Defining the Structure</u> for more details.

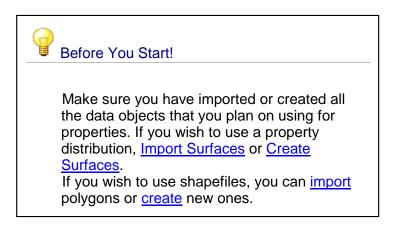
Visual MODFLOW Flex supports various methods for assigning values to hydrogeologic parameters. The method used for defining attributes can be defined on the parameter level, allowing you to use different methods for different parameters. The supported methods include:

- Use Constant Value
- Use Surface Data Object
- Use 3D Gridded Data Object
- Use Shapefile

The following sections provide information on the following topics:

- Defining a New Property Zone
- Assigning Property Parameters
- Editing Property Zones
- Deleting a Property Zone

Creating New Property Zone



Before you can create a property zone, you must have already defined horizons for the conceptual model. For more information, see <u>Defining the Structure</u>.

To define a new property zone, follow the steps below:

- Enter a Name and Description (optional) for the property zone in the Name and Description fields, respectively.
- Select the method by which the property zone geometry will be defined. There are two
 options: Use Structural Zone(s) and Use Polygon Data Object.
- When <u>converting</u> your conceptual model to a numerical model, property zones defined using polygon data objects will take precedence over those defined using structural zones; so that where they overlap, the numerical model will include those values defined by the polygon-based property zone. If one ore more polygon-based zones overlap, the polygon-based zone defined *most recently* will take precedence over any previously defined zone(s).

Using Structural Zone(s)

This method allows you to create a property zone from existing structural zones in your conceptual model, i.e., zones generated from horizons.

Create New Property Zone Method Use Structural Zone(s) Use Polygon Data Object			Sele	Struc	nore stru tural Z	uctural zone: ones	S	_	operty Zones Property Zone 1	
Name										
Propert	ty Zone 1									
Descrip	otion									
										Save
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Condu	uctivity (Kx, Ky,	-							_	
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Condu		-		~	Value 0.0001	•	Object		~	
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- Click on the [Use Structural Zone] button as shown above.
- Select a zone from the Model Explorer tree (under the Zones node), and then click the

button to insert the zone in the Structural Zones field.

- Click the 🖽 Add button to add and combine structural zones.
- Apply to all... button allows you to apply property attribute values for all polygons at once.
- Proceed to <u>Defining Property Zones</u>

Using Polygon Data Object

This method allows you to define a property zone using both a structural zone and a polygon data object. The polygon data object is used to define the horizontal extent of the property zone and therefore must be fully contained within the conceptual model boundary. The structural zone is used to define the volume, i.e., the vertical extent of the property zone.

Create	Create New Property Zone Method Use Structural Zone(s) Use Polygon Data Object			Define Horizontal Extent * Select Polygon Data:				Property Zones Property Zone 1 Property Zone 2	
Name Property Zone 2 Description				efine Volume elect the struct		zone			
Group	ty Values of parameters t ictivity (Kx, Ky,		~						Save
	Parameter	Unit	Method		Value		Object	Mapping	
•	Kx	m/s	Constant	~	0.0001			×	
	Ку	m/s	Constant	~	0.0001			¥	
	Kz	m/s	Constant	~	1E-05			~	
									Apply to all

• Select a polygon data object from the Data Explorer, and click the 🖾 button to insert the data object in the Select Polygon Data field.

Please Note: The selected polygon cannot contain multiple parts, overlapping shapes or holes. These features are currently not supported for property zone creation. If your polygon does not meet this criteria, it can be edited using the 2D Viewer editing tools. For more information on this topic, please see "<u>Creating New</u> <u>Data Objects</u>"

- Next, select a structural zone from the Model Explorer tree, and click the button to insert the data object in the Define Volume frame.
- Apply to all... button allows you to apply property attribute values for all polygons at once.

Assigning Property Parameters

Once the geometry has been defined, you can assign parameter values to the property zone.

• Select the group of parameters that will be defined, e.g., conductivity, storage or initial heads. The data input grid below will display the appropriate parameters based on which parameter group is selected. For example, if conductivity is selected, the data

input grid will show the parameters Kx, Ky, and Kz. The data input grid will already be populated with the default values specified in the Project Settings (File > Project Settings...).

 Visual MODFLOW Flex provides various methods for assigning parameter attributes. The available methods include: Constant Value, Use Surface, Use 3D Gridded Data and Use Shapefile (available only when property zone is defined using polygon data object). The type of method used can be specified per parameter. For each parameter in the data input grid there is a combo box in the Method row (shown below).

-	y Values of parameters t	o define						
Conduc	ctivity (Kx, Ky,	Kz)	~					
	Parameter	Unit	Method		Value		Object	Mapping
•	Kx	m/s	Constant	~	4E-06	€		
	Ку	m/s	Constant	~	4E-06	•		
	Kz	m/s	Constant	~	4E-07	\rightarrow		

Each method is described in the following sections.

Constant Value

The Constant Value method is selected by default for each parameter in the data input grid and allows you to specify a spatially constant value for the parameter. If you do not wish to use the default value, enter a new value.

Use Surface

The Use Surface method allows you use an existing surface data object to define spatiallyvariable attribute values. This is ideal if you have a Surfer .GRD or ESRI ASCII GRD file containing parameter values. Follow the steps below:

- Select "Surface" as the method from the combo box. You should then see the button become activated under the "Value" column
- From the Data Explorer, select the desired surface data object
- Click the button to insert this data object into the Object field.

Please Note: The selected surface data object must cover the entire area of the property zone, or else the data object cannot be used.

Use 3D Gridded Data

The Use 3D Gridded Data method allows you to use an existing 3D gridded data object to define spatially-variable attribute values. Follow the steps below:

- Select "3D Grid" as the method from the combo box. You should then see the button become activated.
- From the Data Explorer, select the 3D Gridded data object
- Click the button to insert it into the parameter field.
- Select the desired attribute value from the "Mapping" combo box.

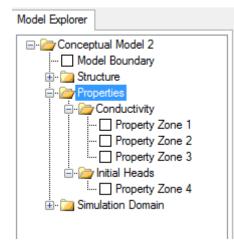
Please Note: The specified 3D Gridded data object must horizontally and vertically overlap the defined property zone geometry, or else the data object cannot be used.

Use Shapefile Attribute

The Use Shapefile method is only available when you define the property zone geometry using a polygon data object. This method allows you to assign an attribute value using an attribute from the specified polygon data object. Follow the steps below:

- If you have not already done so, create the Property Zone <u>Using Polygon Data Object</u>, as described above.
- Select the Use Shapefile Attribute from the method combo box.
- Under Attribute column, the combo box contains all the attributes of the specified polygon.
- Select the desired attribute from the combo box.

Once the property zone attributes have been defined, click the [Save] button to create the property zone. Once created, the property zone is added to the Model Explorer tree under the Properties node and under the appropriate parameter category node.



Overlapping Property Zones

If two or more property zones of the same type overlap (i.e. occupy the same space in 3D), then the following rules of preference will be applied when assigning property values to the discretized numerical model during model conversion:

- Property zones defined by polygon will take precedence over those defined by structural zones, so where these overlap, the model will include the values defined by the polygon
- If two or more polygon-based property zones overlap, the zone defined *most recently* will take precedence over previously defined zones.
- If two or more structural-zone based property zones overlap, the zone defined most recently will take precedence over previously defined zones.

7.6 Defining Boundary Conditions

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Node Explore Severity Severity Severit	Define Wall Boundary Condition	
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At this step, define the boundary conditions for the conceptual model.

Quick Overview

Instructions	Define hydrological boundaries (sources/sinks) for the model
Pre-requisites:	 Structural Zones have been created. Property Zones have been created. You have imported and/or created the data objects you want to use for defining boundary conditions. For example, polylines for the geometry or Surfaces or time schedule for defining the attributes.
Result:	A "conceptual" boundary condition object is created

Next Steps: • Create Finite Difference Grid,

- Create Unstructured Grid, or
- <u>Create Finite Element Mesh</u>

Background

Every conceptual model requires an appropriate set of boundary conditions to represent the system's relationship with the surrounding systems. In the case of groundwater flow model, boundary conditions will describe the exchange of flow between the model and the external system. The following types of flow boundary conditions are supported in the conceptual modeling workflow:

- Specified Head
- River
- General Head
- Drain
- Recharge
- Evapotranspiration
- Lake
- Specified Flux
- Pumping Well
- Wall (Horizontal Flow Barrier)
- Surface water networks (SFR/LAK)

Most of the listed boundary condition types are simple boundary conditions which are specified for one or more model cells with a set number of input conditions as constant values or over a schedule of stress periods, these are considered to be so-called "standard" boundary conditions. Other boundary condition types, such as pumping wells, walls, and surface water networks are more complex in that they require additional inputs or involve more conceptual complexity than assigning values to conceptual point, polyline, or polygon shapes. These specific boundary condition types each have their own workflow steps in the Conceptual Modeling workflow to accommodate their unique complexities.

Please Note: Wall and Surface Water Network boundary conditions are not supported when using LGR or unstructured grids.

Defining Boundary Conditions

In Visual MODFLOW Flex, the boundary condition types are separated into the following categories:

- <u>Boundary Conditions</u> (standard) (Constant Head, Rivers, Drains, General Head, Recharge, EVT, etc.)
- Wall (Horizontal Flow Barrier)
- Pumping Wells
- Surface Water Network Workflow

Modifying Boundary Conditions

From the Model Explorer tree, right-click on the desired boundary condition, and select Edit Boundary Condition... from the pop-up menu.

The Edit Boundary Condition dialog box will display on your screen, allowing you modify the input parameters for the boundary condition. For more information on defining parameter attributes, please refer to "Boundary Conditions Overview" section

Once modifications have been made to the input parameters, click the [Finish] button to save the changes.

Deleting Boundary Conditions

To delete a boundary condition, follow the steps below:

- From the Model Explorer tree, right-click on the desired boundary condition and select Delete from the pop-up menu.
- You will prompted with a confirmation message. Click the [Yes] button to delete the boundary condition.



Please be aware that there is no undo function to recover a deleted boundary condition. Please exercise caution when deleting boundary conditions.

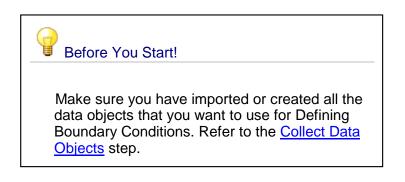
Parameters for Transport Boundaries (Sinks/Sources)

If you need to include contaminant transport in your model, then the species concentrations for transport sinks/sources must also be defined while you create your conceptual boundary conditions. By default, species concentrations will be undefined when you create a new boundary condition. An undefined value is identified by the value "-1" for the species concentration (e.g. Conc001, Conc002). If you wish to assign a contaminant mass to a specific boundary condition object, then replace the default -1 value with a representative contaminant concentration.

Limitations

In Visual MODFLOW Flex, you can create boundary conditions in the conceptual model and in the numerical model. When you edit a conceptual boundary condition object, its corresponding numerical representation will not get updated; likewise, when you update a numerical boundary condition, its corresponding conceptual representation will not get updated. Updates to the conceptual model can be transferred to a new numerical model by (re)-<u>converting</u> the Conceptual Model to a specific grid.

7.6.1 Define Boundary Conditions (Lines/Polygons)



Define Geometry

The first step involves selecting the boundary condition type and specifying the location of the boundary condition on the simulation domain.

- From the Select Boundary Condition Type combo box, select the desired boundary condition type. For more information on each boundary condition type including the data requirements for MODFLOW, please see "Boundary Conditions Overview"
- Enter a Name and a Description (optional) for the boundary condition. The specified name will appear in the Model Explorer tree, once the boundary condition is created.
- Next, select where to apply the boundary condition on the simulation domain by selecting an option from the Where to apply on the Simulation Model Domain combo box. The type of options available in this combo box depend on which boundary condition type is selected. The table below summarizes the available options for each boundary condition type:

*	Define Bo	oundary Conditio	on ×
Cons Ni Evap Rech Spec Di Drain Gene Lake River Cons Where i Top	Boundary Condition Type stant Head (Type 1) stant Head (Type 1) potranspiration (Type 3 MODFLOW Only) harge (Type 2) cified Flux (Type 2) fn (Type 3 - MODFLOW Only) eral Head (Type 3 - MODFLOW Only) eral Head (Type 3 - MODFLOW Only) trope 3 - MODFLOW Only) r (Type 3 - MODFLOW Only) to connect on the Simulation Model Domain to connect on the Simulation Model Domain metry select a polyline or polygon from Data Explorer		Show >> Help Choose the desired boundary condition type from the list, and define a name and optionally, a description. Define where the boundary condition object should be connected on the simulation model domain; this will determine to what model layer the boundary condition will be translated (Top, Bottom, Intermediate). You must then select a polygon or polyline to define the boundary condition geometry. Select the Sides option if you wish to define a boundary condition to the side face of the simulation model domain. For this option, supported boundary condition types are Specified Head, General Head, and Specified Flux
		<< Back N	ext >> Cancel Help

	Тор	Bottom	Side	Intermedi ate
Constant Head	\checkmark			
River				
General Head				
Drain	\checkmark			
Recharge				
Evapotranspi ration	\checkmark			
Lake				
Specified Flux	\checkmark	V		V
Constant Concentratio n	V	V		

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Boundary conditions can be applied to the top, bottom, intermediate layers or sides of the simulation model domain, using imported or digitized Polygon or Polyline data objects, or by manually selecting the sides of the simulation domain using an interactive 3D Viewer.

Each option is described below:

- **Top**: Selecting this option will apply the boundary condition to the top layer of the simulation domain.
- **Bottom**: Selecting this option will apply the boundary condition to the bottom layer of the simulation domain.
- **Side**: Selecting this option will allow you to apply the boundary condition to a single side or combination of sides of the simulation domain. When this option is selected, you will be required to define the geometry of the boundary condition by selecting the desired sides of the simulation domain using an interactive 3D Viewer. For more information on how to do this, please see "Defining Boundary Condition Geometry (Sides)" section
- Intermediate: Selecting this option will allow you to assign the boundary condition to an intermediate model layer within the simulation domain, by specifying a Connection Elevation value. Upon translation, Visual MODFLOW Flex will assign the boundary condition to the appropriate model layer based on the defined connection elevation value.

The next step is to define the geometry of the boundary condition. Boundary conditions that are applied to the top, bottom or intermediate layers can be defined by using a Polygon (areal) or Polyline (linear) data object from the Data Explorer.

- From the Data Explorer, select the polygon or polyline data object that represents the geometry of the boundary condition
- Click the button to insert the data object into the Select a polyline or polygon from the Data Explorer field.

Please Note: Some boundary conditions only support one type of geometry, either polygon or polyline.

Polygons and polyline data objects that extend beyond the model domain must be "clipped" before they can be used to define boundary conditions. Polygons and polylines can be clipped using the "clip to polygon" data operations, which can be accessed in the data object settings (right-click on the polygon or polyline in the Data Explorer, and select Settings... from the pop-up menu). For more information on data object operations, please see "Performing Operations on Data" section.

• Click the [Next] button to proceed to the next step.

For boundary conditions that are to be applied to the Side(s) of the simulation domain, Visual MODFLOW Flex allows you to define the geometry by selecting the appropriate side(s) using an interactive 3D Viewer window. This process is described in "Defining Boundary Condition Geometry (Sides)" section

If you select a polygon data object to define the geometry of the boundary condition, the next step is defining boundary condition parameters. Please skip to "Defining Boundary Condition Parameters" section for information on this topic.

If you select a polyline data object to define the geometry of the boundary condition, the next step is defining zones for the selected polyline. This procedure is described in the following section.

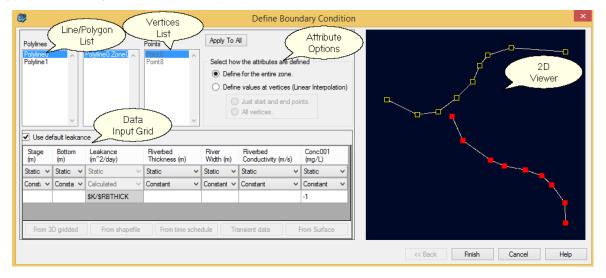
Define Attributes

Visual MODFLOW Flex provides various methods for assigning parameter values to boundary conditions. Each parameter in the boundary condition can be set to Constant or Transient, and values can be assigned using attributes from various imported data objects. The available methods for assigning attributes include:

Parameter values must be entered in the units defined in the project settings. To read more about the project settings, please see "Units" section in the project settings.

Once the geometry has been defined (see previous sections), the next step is to define the boundary condition parameters. Although each boundary condition type requires a different set of parameters, the data input windows each have similar features and functionality. For information on required parameters for each boundary condition, please see the appropriate heading under "Boundary Conditions Overview" section.

A typical boundary condition data input window is shown below:



Select the Method for Defining Attributes (Polylines Only)

For polylines, there are two ways in which you can assign attributes to the boundary condition geometry:

- Define for the entire zone (default): This option allows you to assign boundary condition data to the entire zone.
- Define values at vertices : This option allows you to assign boundary condition data to the vertices along the zone (line), and then during translation, linear interpolation is

used to determine the parameters for the cells that fall between the specified vertices. With this method, there are two options:

- Define Start and End Points: This option allows you to define the attribute value only at the first and last vertex of a zone.
- All Vertices: This option allows you to define attribute values for each vertex in a zone (first, last and all intermediate vertices).

Specifying Boundary Condition Data

Boundary condition data can be specified by using the Data Input Grid. Each column in the data input grid represents a required attribute for the selected boundary condition. For more information on the required parameters for each boundary condition, please see the appropriate section under "Boundary Conditions Overview"

»		D	efine Boundary	Condition		×	
		Zones	Points Point 7	Defin Defin	All w the attributes are define e for the entire zone. e values at vertices (Lin) Just start and end poin) All vertices.	near Interpolation)	
✓ Use de Stage (m)	Bottom (m)	Leakance (m^2/day)	Riverbed Thickness (m)	River Width (m)	Riverbed Conductivity (m/s)	Conc001 (mg/L)	
Static 🗸	Static	✓ Static	Static	Static V	Static 🗸	Static 🗸	
Const: 🗸	Consta	 Calculated 	Constant N	Constant 🗸	Constant 🗸	Constant 🗸	
		\$K/\$RBTHICK				-1	
From 3	From 3D gridded From shapefile From time schedule Transient data From Surface << Back Finish Cancel Help						

Attribute data must be defined for feature (polygon or polyline) in the boundary condition object. Simply select the feature for which attributes are to be defined from the Feature List (the selected line or polygon will be highlighted yellow in the adjacent 2D Viewer preview), and then define the attribute data in the Data Entry Grid. Repeat this process for other features in the selected data object.

Please Note: Attribute data must be defined for all features (polylines or polygons) in the selected data object, in order to complete the creation of the boundary condition.

• [Apply to All]: use this option (located in the top middle portion of the window) to apply the current parameter values/methods, or mapping for the selected polyline (or polygon) to all other polylines (or polygons) in the selected data object. Useful when you have 10's or 100's of features in one data object, and they all reference a common data source (eg. a surface) or a constant value.

For polylines only, it is possible to define attributes at line vertices. In this case, the Points List will become available, where you can select the vertices that comprise the selected zone. For more information on assigning attributes to points, see "Select the Method for Defining Attributes (Polylines Only)" section.

3		De	efine Boundary	Condition		×	
Polylines Zones Points Apply To All Show >> Polyline0 Polyline0.Zone0 Point7 Select how the attributes are defined Select how the attributes are defined Polyline1 Define for the entire zone. Define for the entire zone. Define values at vertices (Linear Interpolation Just start and end points. Just start and end points. All vertices.					ned near Interpolation)		
✓ Use de Stage (m)	fault leakan Bottom (m)	ce Leakance (m^2/day)	Riverbed Thickness (m)	River Width (m)	Riverbed Conductivity (m/s)	Conc001 (mg/L)	
Static 🗸	Static 🗸	Static 🗸	Static V	′ Static ∨	Static 🗸	Static 🗸	
Const: 🗸	Consta 🗸	Calculated V	Constant v	Constant 🗸	Constant 🗸	Constant 🗸	
		\$K/\$RBTHICK				-1	
From 3	From 3D gridded From shapefile From time schedule Transient data From Surface << Back						

For each attribute in the Data Input Grid, there are two combo boxes.

The combo box in the first row allows you to set an attribute as Static (Steady-State) or Transient (conditions change over time). When one or more parameters are set to Transient, the Transient Data button will become active. When selected, the Transient Data window will launch (shown below).

())			Provide Tr	ansient Data		-		<
							▲槽	•橿
	Start	End	Stage					
					ОК] [Cancel	

The Transient Data dialog allows you to define the stress periods and values for all the attributes in the boundary condition that have been set as "Transient".

- Click the Add Row button to add a new row to the table.
- Enter a Start and End time, and a Value for each transient attribute.
- Press the [Enter] button on your keyboard.
- Repeat for additional stress periods.
- Click [OK] to save the transient data.

The second combo box provides different methods for assigning attribute values to the boundary condition.

The contents shown in this combo box depend on the attribute type, i.e., not all methods are available for every attribute. The available methods may include:

- Constant Value
- Use Surface
- Use Shapefile
- Use 3D Gridded Data
- Use Time Schedule (Transient only)

Each method is described below:

Constant Value

The constant value method allows you to define a single value for the entire zone. Upon translation, each grid cell comprising the boundary condition zone will be assigned the specified constant value.

When this method is selected (default), simply enter the desired attribute value in the Data Entry Grid.

Please Note: The values for each constant value attribute should be entered in the same units as defined in the Project Settings.

From Surface

This method allows you to define boundary condition attributes using an existing Surface data object. Upon translation, attribute values are calculated from the specified surface data object. A surface data object can be useful for defining an elevation attribute, i.e., River Stage, Constant Head, Lakebed Bottom etc.

Please Note: The surface data object must cover the entire conceptual model domain area.

When this method is selected, click the [From Surface] button to launch the Static Data Control dialog (shown below).

3	Provide Surface Data	-	□ ×
Stage			
		ОК	Cancel

To specify a surface data object,

- Select the desired surface from the Data Explorer.
- Click the button to insert the surface data object into the attribute field.
- Repeat for other attributes that have been assigned this method.
- Click the [OK] button.

From Shapefile

The method allows you to use Shapefile attributes for defining boundary condition attributes (for example River stage, bottom, riverbed thickness, river width and riverbed conductivity or Constant Head starting head and ending head).

- Select the "Use Shapefile" method from the combo box
- Click the Use Shapefile button to launch the Shapefile dialog; as shown below:

۲	Provide Shapefile Attributes -							
	Stage	River Width	Riverbed Conductivity					
•	¥	¥	¥	*	¥			
	OK Cancel							

or

۲	Provide Shapefile Attributes – 🗆 🗙					
	Starting Head	Ending Head				
•	×	~				
				01/		
				OK	Cancel	

- The combo box contains all the attributes of the specified polygon used to define the horizontal geometry of the boundary condition.
- Select the desired attribute from the combo box, and then click the [OK] button to close the dialog box.

From 3D Gridded Data

This method allows you to use spatially-variable attributes from a 3D Gridded data object for defining a boundary condition attribute. When this method is selected, the Use 3D Gridded Data button will become active. When selected, the 3D Gridded Data dialog will launch.

- From the Data Explorer, select the desired 3D Gridded data object
- Click the button to insert it into the Select 3D Gridded Data Object field.
- Once selected, the data object's attributes are listed in the combo box below.
- Select the desired attribute from the combo box, and then click the [OK] button to close the dialog box.

Please Note: The specified 3D Gridded data object must horizontally and vertically overlap the defined property zone geometry, or else the data object cannot be used.

Use Time Schedule

This method allows you to use a time-schedule data object for defining the stress periods and values of a transient attribute. When this method is selected, click the Use Time Schedule button to launch the Time Schedule dialog.

*	Provide Time Schedule	Data –	□ ×
Select	time schedule object		
•	Stage		
		OK	Cancel

- From the Data Explorer, select the desired time schedule data object
- Click the button to insert it into the Select Time Schedule Object field.
- Once selected, the data objects attributes are listed in the combo box below.
- Select the desired attribute value from the combo box, and then click the [OK] button to close the dialog box.

Use Default Leakance

The Use Default Leakance option is used to calculated the leakance value for River, Drain, Lake and General Head boundary conditions using a mathematical expression containing array variables (see the section "Using Mathematical Formulas and Array Variables in the Visual MODFLOW Flex User's Manual for more information). If the Use Default Leakance option is selected, the leakance value will be calculated using a default formula associated with each boundary condition type. If this option is not selected, a leakance value will need to be entered manually.

The advantage of using the default leakance formula to calculate the leakance value for the group of grid cells is that each grid cell will be assigned a leakance value proportional to the size of the grid cell.

Linear Interpolation Explained

When the Define values at vertices option is selected, two sets of boundary condition data are required; one set for the grid cell at the Start Point of the line (or line segment), and one set for the grid cell at the End Point of the line (or line segment). The boundary condition data for the grid cells between the Start Point grid cell and the End Point grid cell will be linearly interpolated between these two points using the formula below:

$$x_{i} = x_{sp} + (x_{sp} - x_{ep}) \times \left(\frac{\$TVAR_{1,i}}{\$LENGTH}\right)$$

where:

 x_i is the boundary condition parameter value at the ith grid cell along the polyline

 x_{sp} is the boundary condition parameter value at the Start Point of the polyline

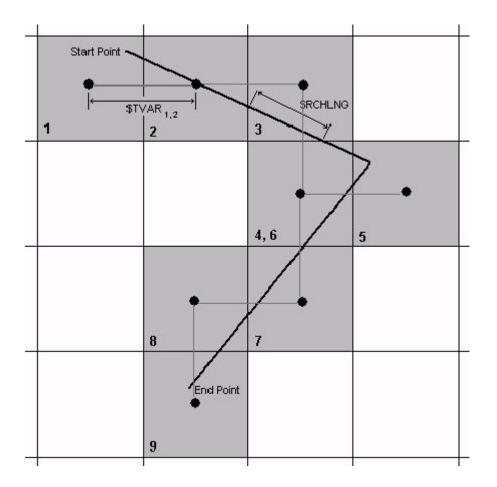
 x_{ep} is the boundary condition parameter value at the End Point of the polyline

 x_{ep} is the boundary condition parameter value at the End Point of the polyline

 $TVAR_{1,i}$ is the cumulative length of the line at the ith grid cell along the line, as measured from the center of the Start Point grid cell through the center of each successive grid cell along the line, also known as the Manhattan or <u>taxicab</u> distance (see figure below).

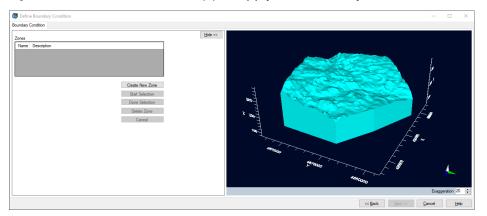
LENGTH is the total length of the line, as measured from the center of the Start Point grid cell through to the center of the End Point grid cell (see figure below).

When the line is digitized from the Start Point to the End Point, each grid cell is numbered in sequence according to the order in which the line passes through each cell. If the line passes through the same grid cell twice, the grid cell will be numbered twice as seen for grid cell "4" and "6" in the following figure. As a result, the parameter value calculated for "grid cell #6" will overwrite the parameter value calculated for "grid cell #4".



7.6.2 Define Boundary Conditions to Sides

If you choose to apply the boundary condition to the Sides of the simulation domain, click the [Next] button to select which side(s) to apply the boundary condition to.



Applying boundary conditions to the sides of the simulation domain is accomplished by manually selecting the desired sides using an interactive 3D Viewer window.

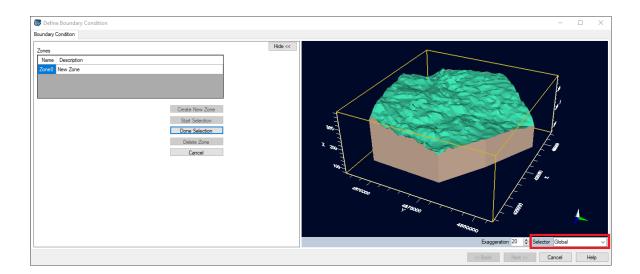
• Click the [Show] button to display the interactive 3D Viewer.

The interactive 3D Viewer behaves just like any other 3D Viewer. You can zoom in and out (using the mouse wheel), rotate and move the displayed simulation domain using your mouse. You can also change the color of the background, show/hide the axis, and change the vertical exaggeration.

Creating a New Zone

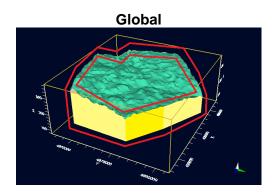
To create a new zone, follow the steps below:

- Click the [Create New Zone] button. A new row will be added to the Zones table. Here you can change the zone Name and Description, as desired.
- Click the [Start Selection] button. A new combo box called Selector will be added to the bottom of the interactive 3D Viewer (indicated below).

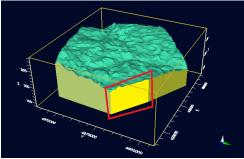


From the Selector combo box, select one of the following options:

- Global: Select all sides around the entire simulation domain.
- Vertical: Select one or more area(s) between two edges of the simulation domain bounding polygon, spanning the entire height of the simulation domain.
- Horizontal: Select the area(s) between two horizons, around the entire simulation domain (subject to pinchouts).
- **Facets**: Select one or more area(s) that are bounded on the sides by edges of the simulation domain, and bounded at the top/bottom by horizons.

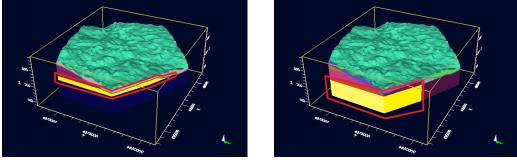


Vertical



Horizontal

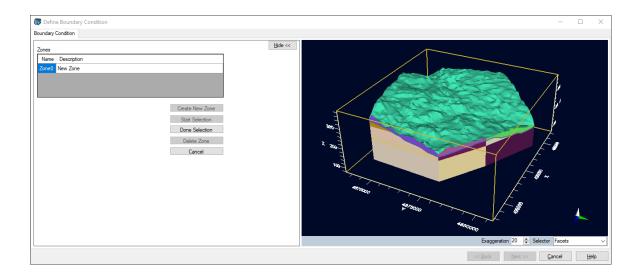
Facets



Using your mouse, click on the simulation domain in the 3D Viewer, and select the appropriate sides for the boundary condition. When a side is selected, it will become highlighted.



You can select multiple verticals, sides, or facets by holding down the [CTRL] key on your keyboard while adding to your selection using left click(s) of your mouse.



Once the desired areas have been highlighted, click the [Done Selection] button to save the selections.

Repeat the steps above to create additional zones.

When you are finished, click Next to define the attributes; for more details, see <u>Define</u> <u>Boundary Conditions (Lines/Polygons)</u>

7.6.3 Define Pumping Wells

At this step, you can define well boundary conditions.

😻 Add Wells	-
Well Object Name: Well Well Model: WEL Vell Model: WEL	Data To Display Active Well: <none> Display Format Screens Elevation Measured Depths </none>
Well Heads	Screens
+ □= = × = 6	- = = × = =
Name X Y Zmax Zmin Active	Show as Relative Times Reference Time 1/1/2000 12:00 AM Pumping Schedule Reference Time 1/1/2000 12:00 AM
	Apply OK Cancel

Quick Overview

Instructi ons:	Select a wells data object to be used as wells in the conceptual model
Pre- requisit es:	Boundary Conditions are created You have imported a wells data object, with screens and pumping schedule information.
Result:	A Conceptual Wells Boundary Condition object is created
Next Steps:	 <u>Create Finite Difference Grid;</u> <u>Create Unstructured Grid;</u> or <u>Create Finite Element Mesh</u>

Adding a new Pumping Well Boundary Condition

To add a are two ways to add new pumping well boundary condition, follow the steps below:

- Add Wells \times Display Format Data To Display Active Well: <None> Well Model: WEL Well Object Name: Well Elevation Select Raw Wells Data Object or Drag & Drop Measured Depths \Rightarrow Find: Vertical Well Heads 🕂 💷 🛤 🗶 🐚 🖺 + = = X = 6 Zmax Name X Y Zmin Active Reference Time 1/1/2000 12:00 AM Show as Relative Times Pumping Schedule + = = X = 6 Apply OK Cancel
- Click on the Define Pumping Wells button; the following window will appear:

Adding a Well Object

- · Select a pumping wells data object from the Data Explorer
- Click the button to insert the data object into the Select Wells Data Object field. The wells should then show in the table.

Each pumping well must satisfy the following requirements in order to be deemed valid:

- The pumping well must located within the simulation domain.
- A screen must be defined for the pumping well
- A pumping schedule must be defined for the pumping.

Wells that do not meet these requirements will not be included. For information on defining well data, i.e., screens, pumping schedules, please see "<u>Well Table</u>" section

Visual MODFLOW Flex will then add the boundary condition under the Boundary Condition node in the Model Explorer tree. For more information about wells, please see the <u>Theory</u> <u>section</u> on wells.

7.6.4 Define Wall (HFB)

Visual MODFLOW Flex supports the Horizontal Flow Barrier (HFB) Package included with MODFLOW. The Horizontal-Flow-Barrier (HFB) Package, or Wall Boundary as it is referred to in Visual MODFLOW Flex, was developed to simulate thin, vertical, low-permeability features that impede the horizontal flow of groundwater. This package allows such features to be simulated without the need to reduce grid spacing in an excessive number of model cells, thus enhancing model efficiency. These features are approximated as a series of horizontal flow barriers conceptually situated on the boundaries between adjacent cells in the finite difference grid.

The key assumption underlying the HFB Package is that the thickness of a barrier is negligibly small in comparison to the horizontal dimensions of the cells in the grid. Barrier width is not explicitly considered in the Package, but is represented in MODFLOW as a hydraulic characteristic defined as barrier hydraulic conductivity divided by barrier thickness.

The HFB Package requires the following information as input for each cell containing this boundary condition:

- (I1, J1): Row and column number of grid cell on one side of the barrier.
- (I2, J2): Row and column number of grid cell on the other side of the barrier.
- Hydchr: Hydraulic characteristic of the barrier (equivalent to hydraulic conductivity of the barrier divided by the width of the barrier).

Wall Boundaries are currently not supported for MODFLOW-6, MODFLOW-USG, MODFLOW-LGR numerical models, or MODFLOW-2000/2005 grids using a Uniform or Semi-Uniform vertical layering approach.

Walls can be defined in the Conceptual Model workflow, or in existing numerical models using structured grids (excluding MODFLOW-LGR). The behaviour for Walls is similar to other boundary conditions in Visual MODFLOW Flex; if you create this object in the Conceptual Model workflow, then the numerical realization of the Wall will be created after you run "Convert to Numerical Model" steps. If you "Assign" a wall in a numerical model, then Visual MODFLOW Flex will create the conceptual object and also create the numerical wall representation at the same time.

In Visual MODFLOW Flex, Wall objects are assembled using existing data objects in the Data tree and from Conceptual Model. Horizontal Flow Barriers (or Walls) are assigned by using polyline objects to define the spatial extent, and Horizons to define the upper and lower extents.

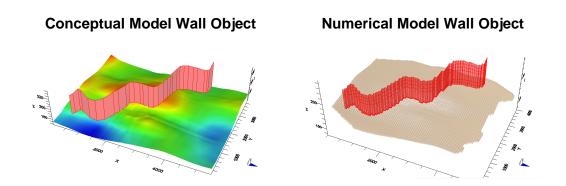
Define Wall Boundary Condition
Name:
Wall
Select Polyline(Drag from Model Tree)
Select Horizons(Drag from Model Tree)
Top Horizon:
Bottom Horizon:
Define Attributes
Conductivity:
m/s
Thickness:
OK Cancel Help

How to Create a Wall Boundary

- 1. Select "Define Wall Boundary" from the conceptual model, or select "Assign" option at the Define Boundary conditions step in the numerical model
- Import the desired polyline object, or digitize the desired polyline using the 2D Viewer (see <u>Creating New Data Objects</u> for more details). Note: the polyline data object must contain only one line feature.
- 3. Choose this Wall object from the Data tree
- 4. Click on the button (under Select Polyline) in the Define Wall Boundary Condition window to apply this data
- 5. In the Model Explorer, expand the Model Explorer tree, then expand Structure / Horizons to see a list of Horizons.
- 6. Select a Horizon object from the Model explorer that represents the top location for the wall
- 7. Click on the button (under Top Horizon) in the Define Wall Boundary Condition window to apply this data
- 8. Repeat these steps for the bottom Horizon
- Define the Attributes: Conductivity: The hydraulic conductivity of the barrier wall. Thickness: The thickness of the barrier wall.

10.Click OK when you are finished. The Wall object will appear on the Model explorer, under the Conceptual Model / Boundary Conditions folder. If you created the Wall from within a numerical model workflow, then you will also see an item "Wall". If you created the Wall in the Conceptual Model, then the Wall numerical boundary condition will only show up after you complete the <u>Conceptual to Numerical Model Conversion</u>.

Visual MODFLOW Flex will automatically calculated the appropriate cell faces based on the intersection point of the polyline and spanning through the appropriate model layers.



Edit Conceptual Model Wall Object

You can edit the attributes for a Conceptual Model Wall object by right-clicking on this item in the Model Explorer, and selecting "Edit Boundary Condition". Please note that if you change the attributes, you need to re-run the Conceptual Model to Numerical Model conversion in order to re-generate the numerical model Wall object(s).

Edit Numerical Model Wall Attributes

You can edit the attributes for a Numerical Model Wall object by right-clicking on this item in the Model Explorer, and selecting "Edit Attributes...". The attributes will load as a CSV file in either Excel or Notepad (or other text editors if you have associated a different program to .CSV file extensions). Make the desired changes to the values, then save and close the file. When you are finished and wish to update the Wall object with your edits, right-click on this item in the Model Explorer and select "Reload Attributes..." to refresh the values in the numerical model.

7.6.5 Theory

Every model requires an appropriate set of boundary conditions to represent the system's relationship with the surrounding systems. In the case of a groundwater flow model, boundary conditions will describe the exchange of flow between the model and the external

system. In the case of a mass transport model, the boundary conditions will also describe the exchange of solute mass between the model and the external system.

The following sections present an overview of the boundary condition packages supported in Visual MODFLOW Flex. Each section includes a brief description of the boundary condition, including the input data required by MODFLOW and the supported data objects for defining the boundary condition geometry. The following boundary conditions are discussed in this section:

- <u>Well</u>
- o Wells (WEL)
- Multi-Node Wells (MNW1/MNW2)
- Constant Head (CHD)
- <u>River</u> (RIV)
- <u>General Head</u> (GHD)
- Drain (DRN)
- Streamflow-Routing (SFR2)
- Recharge (RCH)
- Evaporation (EVT)
- Lake (LAK)
- <u>Specified Flux</u> (FHB)
- Time-varying Material Properties (TMP)
- <u>Unsaturated Zone Flow</u> (UZF)
- Mass Source Loading (SRC)

Well

There are several different types of Well boundary condition supported in Visual MODFLOW Flex that each include different conceptualizations of groundwater withdrawals/injections via wells via distinct boundary condition packages:

wen Types								
Well Model	WEL	MNW1	MNW2					
Engines	Engines							
MF-2000	$\mathbf{\nabla}$	\checkmark						
MF-2005								
MF-NWT								
MF-LGR								
SEAWAT	\checkmark							
MF-SURFACT								
MF-USG								

Well Types

WEL Package

The well (WEL) package is the simplest boundary condition used to simulate wells in MODFLOW. In the WEL package, wells (and other features) are conceptualized as points sinks that withdraw water from or sources that add water to the model at a constant rate during a stress period, where the rate is independent of both the cell area and head in the cell.

The MODFLOW input data for Well cells is stored in the projectname.WEL file. You can define the location for vertical or non-vertical wells (which include the well path and the screen location). When you translate your conceptual model to MODFLOW format, the well screen locations are converted to set of pumping well cells. Another option is to define a specified flux or drain boundary condition in Visual MODFLOW Flex.

Conceptualization in MODFLOW

Visual MODFLOW Flex supports pumping wells with one or more screen intervals along the path of the well bore, including well screens that partially penetrate a model layer. However, it is important to note that the WEL package in MODFLOW does not include any special considerations for multiple well screens or grid cells containing partially penetrating well screens. MODFLOW treats WEL pumping wells as simple flux boundary conditions, such that each grid cell intersecting a well screen is assigned a specified flux that is constant for a given stress period. In a situation where a well is screened across several model layers, Visual MODFLOW Flex uses the length of the well screen intersecting each model layer to determine the proportion of the total well pumping rate assigned to each well grid cell in the model, even though MODFLOW considers a cell to be screened over its entire vertical length, regardless of the length of screen assigned to the cell. The following equation is used to calculate the pumping rate for each grid cell:

$$Q_i = Q_T \frac{L_i K_{x(i)}}{\sum \left(L_i K_{x(i)} \right)}$$

where:

 Q_i is the specified discharge from the ith cell to a particular well in a given stress period

[L3/T]

(1)

 Q_T is the total specified pumping rate for all screens in a particular well in a given stress period [L3/T]

 L_i is the screen length of screen in the ith cell

 $K_{x(i)}$ is the hydraulic conductivity in the x-direction in the ith cell

[L/T]

[L]

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 $\sum (L_i K_{x(i)})$ represents the sum of the products of screen length and hydraulic conductivities in the x-direction of all cell penetrated by the well.

 $[L^2/T]$

The WEL package approach, in which a well screened over one or more cells/layers is represented as a set of independent specified flow rates, fails to take into account the interconnection between various layers provided by the well. One of the most significant problems related to this approach is that MODLFLOW will inactivate cells and their boundary conditions when the water table drops below the bottom of the grid cell (i.e. when the grid cell becomes dry). This automatically reduces the total pumping rate of the well, and may cause the water table to "rebound" and re-activate the well grid cell. This type of on-again-off-again behavior for the pumping well(s) causes the solution to oscillate, and may prevent the model from converging to a solution. In the event the model does converge to a solution, the model results may be misleading if one or more pumping wells have lower than expected total pumping rates.

Alternately, a multi-layer well can sometimes be simulated by means of a vertical column of high permeability cells with a screen at the bottom of the column. In this case, if the top part of the model becomes dry, the total pumping rate is unaffected. This also takes into account the vertical inter-connection between layers. The downside of this approach is that the conductivity contrasts can lead to convergence problems.

The MNW1 and MNW2 packages (described below) provide better representation of wells screened over multiple layers. Both of these packages are able to dynamically redistribute pumping rates to the remaining active grid cells if one or more cells in the screened interval goes dry, thereby more accurately simulating the real-world effects of partial overpumping of a well screened over multiple layers.

Despite the limitations described above, the WEL package includes some advantages over the MNW packages described below, including that it has minimal input data requirements and it is very computationally efficient and stable.

Required Data

In Visual MODFLOW Flex, pumping well boundary conditions in the WEL package are defined using the well data contained in a wells data object. During the boundary condition creation process, you will be required to select a wells data object from the Data Explorer.

A well can only be used if it meets the following requirements:

- The pumping well must be located within the simulation domain
- One or more screens must be defined for the pumping well
- A pumping schedule with at least one stress period must be defined for the pumping well

For information on importing well data, please see "<u>Importing Wells</u>" section. For information on defining well data for existing wells data objects, please see the "<u>Well Table</u>" section

MNW1 and MNW2 Packages

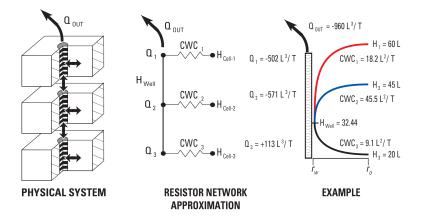
Pumpage from aquifer systems is commonly more complex than the simple considerations included in the WEL package described above. The Multi-Node Well packages (MNW1 and MNW2) were developed to include additional complexities associated with well screens that span multiple layers/cells, including:

- the head in the well is distinct from the head(s) in the neighboring formation,
- pumping is from the entire well, and
- pumping rates may be constrained by the physical limitations of the pump configuration

For example, heads in aquifers that surround a well are likely to vary along the length of a screen, particularly if the well screen penetrates multiple aquifers or has a long horizontal extent. When pumping, recharge, or no user-specified inflow or outflow occurs in wells that are screened across multiple aquifers or in a single aquifer, there can be significant hydraulic effects on the ground-water flow system. The Multi-Node Well packages (MNW1 and MNW2) have been integrated in Visual MODFLOW Flex to help simulate intraborehole flow occurring in wells with screens that span multiple layers. MNW1 was the original implementation by the USGS (Halford and Hanson, 2002) and provided a great deal of flexibility for specifying well input parameters that may change over time. MNW2 provides a somewhat streamlined input structure (Konikow, *et al.*, 2009) and allows for some additional well configurations/processes, most notably those associated with non-vertical wells.

Conceptualization in MODFLOW

Visual MODFLOW Flex supports pumping wells with one or more screen intervals along the path of the well bore, including well screens that partially penetrate a model layer. In the Multi-Node Well packages, the flow rate from the pumping well and heads in the well and adjacent model cells are based on an analogous approximation of resistors in a network:



Source: Halford and Hanson (2002)

$$Q = h_w \sum (CWC_i) - \sum (h_i CWC_i)$$
⁽²⁾

where:

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Q is the total flow rate from the well (positive for injection and negative for withdrawal) [L³/T]

 h_w is the head in the well [L],

 h_i is the head in the formation at model cell i along the well screen(s) [L],

 CWC_i is the cell-to-well conductance at model cell i along the well screen(s) [L²/T]

The cell-to-well conductance in the MNW package is based on the following equations (Halford and Hanson, <u>2002</u> and Konikow, et al, <u>2009</u>):

$$CWC_i = (A + B + CQ_i^{(P-1)})^{-1}$$
(3)

where:

A is the linear formation head-loss coefficient given by $[T/L^2]$:

$$A = \left[\frac{ln\left(\frac{r_o}{r_w}\right)}{2\pi b_i \sqrt{K_{x(i)}K_{y(i)}}}\right]$$

-

(4)

B is the linear well head-loss coefficient given by $[T/L^2]$:

$$B = \left[\frac{Skin_i}{2\pi b_i \sqrt{K_{x(i)}K_{y(i)}}}\right]$$
(5)

C is the non-linear well head-loss coefficient

P is the non-linear well head-loss exponent (1.0 - 3.5, usually 2.0) [L²/T]

 b_i is thickness of the formation in model cell i [L]

 r_o is the effective radius of the rectilinear finite difference cell which is calculated automatically by Visual MODFLOW Flex using equation 6 in Halford and Hanson (2002) [L]

 r_w is the radius of the well screen [L]

 $Skin_i$ is a Skin factor for model cell i, based on the following equation [-]:

$$Skin_{i} = \left[\frac{b_{i}\sqrt{K_{x(i)}K_{y(i)}}}{b_{w(i)}K_{Skin}} - 1\right]ln\left(\frac{r_{Skin}}{r_{w}}\right)$$

(6)

 $K_{x(i)}$ is the hydraulic conductivity of the formation in the x-direction in the ith cell [L/T],

 $K_{y(i)}$ is the hydraulic conductivity in the formation in the y-direction in the ith cell [L/T],

 K_{Skin} is the hydraulic conductivity of the well skin along the borehole [L/T],

 $b_{w(i)}$ is length of the well screen in model cell i [L]

 r_{Skin} is the radius of the well skin [L],

For more information on the development and theory behind these packages, please see the original USGS reports for MNW1 by Halford and Hanson, (2002) and for MNW2 by Konikow, *et al.*, (2009).

Required Data

In Visual MODFLOW Flex, pumping well boundary conditions are defined using the well data contained in a wells data object. During the boundary condition creation process, you will be required to select an existing wells data object from the Data Explorer or create a new one.

Multi-node wells must include the following minimum information:

- The pumping well must be located within the simulation domain
- One or more screens must be defined for the pumping well
- A pumping schedule with at least one stress period must be defined for the pumping well
- · Parameters for well hydraulics

Well Loss parameters

There are several options in the multi-node well packages to define the head loss between the well and the adjacent cells in each of the multi-node well packages. The options and their relevant input variables are presented in the Table 1 and Table 2 below for the MNW1

and MNW2 packages, respectively, while descriptions of the relevant input variables are presented further below.

		Required Input Properties							
Loss Model [*]	MNW1 Option [*]	Rw ** (<i>r</i> _w)	$\frac{\mathbf{Rskin}}{(r_{skin})}$	$\frac{\text{KSkin}}{(K_{Skin})}$	B **	C **	Ρ*	cwc **	CWCDis t **
None	Skin	0							
Thiem	Skin	V	Rw						
Skin	Skin	V							
Linear	Linear	V							
Non-Linear	Non-Linear	V							
Specify CWC	Skin	-cwc						V	

Table 1. Supported MNW1 loss types in Visual MODFLOW Flex

Notes:

* the property is global and specified once for all wells in the MNW1 package

^{**} the property is transient and specified for each well/stress period. Flex will distribute values each to cell intersecting the well screen(s)

		Required Input Properties							
Loss Model [*]	MNW2 Option [*]	Rw ** (<i>r</i> _w)	$\frac{\mathbf{Rskin}}{(r_{Skin})}$	$\frac{\text{KSkin}}{(K_{Skin})}$	B **	C **	Ρ*	CWC **	CWCDis t **
None	None								
Thiem	Thiem								
Skin	Skin		V						
Linear	General					0			
Non-Linear	General						V		
Specify CWC	SpecifyCWC							V	V

Notes:

* the property is static and specified once for each well

^{**} the property is static and specified once for each well. Flex will distribute values to each cell intersecting the well screen(s)

The input variables for the well loss models are as follows:

- **Rw**: Radius of the well screen (L)
- **RSkin**: Radius of the well skin (L)
- KSkin: Hydraulic conductivity of the well skin (L/T)
- B: Linear well loss coefficient
- C: Non-linear well loss coefficient
- P: Non-linear well loss exponent (1.0 to 3.5, default 2.0)
- CWC: cell to well loss coefficient
- CWC Dist: Option for defining how the CWC coefficient is distributed across the cell(s) spanning the screen:
 - o By Cell,
 - o By Screen Cell Thickness,
 - By Screen Cell Transmissivity

Well Performance and Constraints

The multi-node well packages provide input variables that allow you to define conditions on pumping in the well.

Input Parameter	MNW1 [*]	MNW2**
Water Limit	\checkmark	
HLim	V	\checkmark
Href	\checkmark	
QCut	V	V
Qfrcmn	\checkmark	\checkmark
Qfrcmx	V	V

Notes:

 * input variables are transient are specified for each well in each stress period. Flex will distribute values to cell intersecting the well screen(s)
 ** the property is static and specified once for each well

The input variables for the well performance and constraints are as follows:

- WaterLimit: Option to set the reference type for HLim and Href
 - "Water Level": water level constraints are based on the absolute water level in the specified well
 - "Drawdown": water level contraints are based on relative water level in the specified well (drawdown)
- **HLim:** limiting water level in the well (a minimum for discharging wells [Q<0] and a maximum for injection wells [Q>0]. For example, if the head in the well falls below this value in a discharging well, then pumping in the well ceases.
- **Href**: Reference elevation for the limiting water level (HLIM). If the value of HREF is greater than the maximum water level at the beginning of stress period 1, HREF is set to the simulated water level at the location of the head/drawdown-limited well.

- QCut: Option to set pumping rate limit types for Qfrcmn and Qfrcmx, either by absolute rate or by percent
 - o **Qfrcmn**: Pumping rate or fraction (see QCUT) below which pumping will cease
 - Qfrcmx: Pumping rate or fraction (see QCUT) above which pumping will resume/be reactivated

Supported Geometry

Wells in Visual MODFLOW Flex are based on well data objects. For information on importing well data, please see "Importing Wells" section.

For information on defining well data for existing wells data objects, please see the "<u>Well</u> <u>Table</u>" section.

Constant Head

The Specified Head boundary condition, also known as Constant Head in VMOD Flex, is used to fix the head value in selected grid cells regardless of the system conditions in the surrounding grid cells, thus acting as a potentially <u>infinite</u> source of water entering the system, or as an <u>infinite</u> sink for water leaving the system. Therefore, specified head boundary conditions can have a significant influence on the results of a simulation, and may lead to unrealistic predictions, particularly when used in locations close to the area of interest.

During translation, VMOD Flex uses the Time-Variant Specified-Head (CHD) Package provided with MODFLOW. The MODFLOW input data for Specified Head cells is stored in projectname.CHD file.

Unlike most other transient MODFLOW boundary condition packages, the Constant-Head package allows the specified heads to be linearly interpolated in time between the beginning and end of each stress period, such that the specified head for a grid cell may change at each time step within a given stress period. If the simulation is steady-state, the specified starting head value will be used from the first stress period. Note, this is no longer the case, in MODFLOW-6 which only supports single values for each stress period using the basic input method.

Required Data

The Specified-Head package requires the following information for each specified head grid cell for each stress period:

- Start Head: Specified head value at the beginning of the stress period
- Stop Head: Specified head value at the end of the stress period

Supported Geometry

The geometry for Specified Head boundary conditions can be specified using Polylines or Polygons

A Note on Leakance vs. Conductance

Some Type-3 (Head-Dependent Flux) boundary conditions (e.g. river and general head) require defining a conductance parameter (for MODFLOW). Conductance is a numerical parameter representing the resistance to flow between the cell assigned with that boundary condition and the surrounding cells. Conductance between cells is calculated using some average hydraulic conductivity of the cells, the area of the interface between the cells and the distance between the cell centers. The Conductance calculation requires the cell geometry (cell interfaces).

In Visual MODFLOW Flex, when you create a new conceptual boundary condition, this is done using shapes: polyline, polygon, and side faces. At this point, there is no notion of cell geometry, as a result, the conductance cannot be calculated since the cell face area cannot yet be calculated. For this reason, you are asked to define "Leakance" instead of "Conductance". Leakance is a conceptual (hydrogeologic) term, and is expressed per unit area (if the conceptual boundary condition object is a polygon) or per unit length (if the conceptual boundary condition object is a polyline).

When you create the boundary condition, the Leakance can be calculated based on other defined parameters, or it can be explicitly defined.

When you look at the numerical representation (cell realization) of the boundary condition, you will see "Conductance" as the parameter, since this value can be calculated based on the intersecting cell geometry. For a boundary condition assigned with a polygon or side face, the Leakance is multiplied by the cell area, in order to get Conductance. For a boundary condition assigned with a polyline, the Leakance is multiplied by the length of the line that intersects the cell, in order to get the Conductance.

More details on this can be found at:

http://water.usgs.gov/ogw/modflow/MODFLOW-2005-Guide/index.html?frequently_asked_questions.htm.

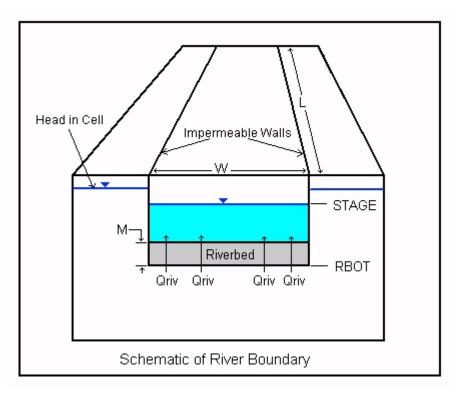
River

The MODFLOW River Package simulates surface water/groundwater interaction via a seepage layer separating the surface water body from the groundwater system. VMOD Flex

uses the River Package included in MODFLOW. MODFLOW input data for River grid cells is stored in *projectname.RIV* file.

Conceptualization in MODFLOW

The River boundary condition is a simple conceptualization of surface water features used to simulate the influence of a surface water body on the groundwater flow system. Surface water bodies such as rivers, streams, lakes and swamps may either contribute water to the groundwater system, or act as groundwater discharge zones, depending on the hydraulic gradient between the surface water body and the groundwater system. The conceptualization of rivers (or other surface water features that this boundary condition is used to represent) is represented as a seepage layer of bed sediments that is assumed to be a flat bottom, with no seepage through the sides of the channel as shown below:



The RIV package approach, fails to take into account the mass balance in the overlying surface water feature and can supply or remove an infinite amount of water to/from the groundwater system. The can produce non-physical results with unexpected amounts of water being exchanged between the groundwater and surface water system both locally and regionally in the model.

The Streamflow-Routing (SFR) package (described below) provides a better representation of river systems, and includes conceptualizations of flow within and between stream reaches, which are entirely ignored in the RIV conceptualization

Required Data

The MODFLOW River Package input file requires the following information for each grid cell containing a River boundary;

- **River Stage**: The free water surface elevation of the surface water body. This elevation may change with time.
- **Riverbed Bottom**: The elevation of the bottom of the seepage layer (bedding material) of the surface water body.
- **Conductance**: A numerical parameter representing the resistance to flow between the surface water body and the groundwater caused by the seepage layer (riverbed).

The Conductance value (C) may be calculated from the length of a reach (L) through a cell, the width of the river (W) in the cell, the thickness of the riverbed (M), and the vertical hydraulic conductivity of the riverbed material (K) using the following formula:

$$C = \frac{K \times L \times w}{M}$$

(7)

For situations where the River package is used to simulate lakes or wetlands, the L and W variables would correspond to the X-Y dimension of the River boundary grid cells. When a River boundary condition is assigned, the Use default Leakance option is automatically selected.

If the Use default Leakance option is selected, the River boundary condition requires the following data:

- River Stage: The free water surface elevation of the surface water body. [L]
- **Riverbed Bottom**: The elevation of the bottom of the seepage layer (bedding material) of the surface water body. [L]
- Riverbed Thickness: Thickness of the riverbed (seepage layer) [L].
- Leakance: A numerical parameter representing the resistance to flow between the surface water body and the aquifer (this field is read-only and is calculated using the formula described below). [L²/T or L/T, see below]
- Riverbed Kz: Vertical hydraulic conductivity of the riverbed material. [L/T]
- River Width: Width of the river. [L]

When a polyline is used to define the river geometry, the default conductance formula is as follows:

$$\$COND = \frac{\$RCHLNG \times \$WIDTH \times \$K \times \$UCTOCOND}{\$RBTHICK}$$

(8)

When a polygon is used to define the river geometry, the default conductance formula is as follows:

$$COND = \frac{DX \times DY \times K \times UCTOCOND}{RBTHICK}$$

where:

\$COND: is the Conductance

\$RCHLNG: is the reach length of the river line in each grid cell

\$WIDTH: is the River Width in each grid cell

\$K: is the Riverbed Kz

\$UCTOCOND: is the conversion factor for converting the \$K value to the same L and T units used by \$COND. \$UCTOCOND is automatically calculated by Visual MODFLOW Flex.

\$RBTHICK: is the Riverbed Thickness

\$DX: is the length of each grid cell in the X-direction

\$DY: is the length of each grid cell in the Y-direction

If the "Use default Leakance" option is turned off, the fields used for calculating the River Leakance value (Riverbed Thickness, Riverbed Kz, and River Width) are removed from the table, and the Leakance field becomes a writable field where a value may be entered.

Supported Geometry

The geometry for River boundary conditions can be specified using polylines or polygons

General Head

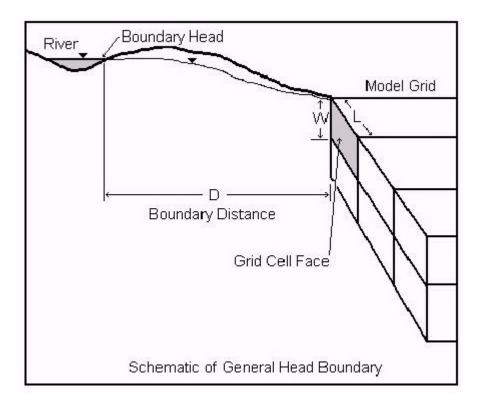
VMOD Flex supports translation of the General-Head Boundary Package included with MODFLOW. The MODFLOW input data for General-Head grid cells is stored in the *projectname.GHB* file.

Conceptualization in MODFLOW

The function of the General-Head Boundary (GHB) Package is mathematically similar to that of the River, Drain, and Evapotranspiration Packages. Flow into or out of a cell from an external source is provided in proportion to the difference between the head in the cell and the reference head assigned to the external source. The application of this boundary

(9)

condition is intended to be general, as indicated by its name, but the typical application of this boundary condition is to represent heads in a model that are influenced by a large surface water body outside the model domain with a known water elevation. The purpose of using this boundary condition is to avoid unnecessarily extending the model domain outward to meet the element influencing the head in the model. As a result, the General Head boundary condition is usually assigned along the outside edges (sides) of the simulation model domain. This scenario is illustrated in the following figure.



The primary differences between the General-Head boundary and the Specified Head boundary are:

- the model solves for the head values in the General-Head grid cells whereas the head values are specified in Constant Head cells.
- the General-Head grid cells do not act as infinite sources of water whereas Specified Head cells can provide an infinite amount of water as required to maintain the specified head. Therefore, under some circumstances, the General-Head grid cells may become dry cells.

Required Data

The General-Head Boundary Package requires the following information for each General-Head grid cell:

- Stage: This is the head of the external source/sink. This head may be physically based, such as a large lake, or may be obtained through model calibration.
- Conductance: The is a numerical parameter that represents the resistance to flow between the boundary head and the model domain.

In contrast to the River, Drain, and Evapotranspiration packages, the General Head package provides no limiting value of head to bind the linear function in either direction. Therefore, as the head difference between a model cell and the boundary head increases/decreases, flow into or out of the cell continues to increase without limit. Accordingly, care must be used to ensure that unrealistic flows into or out of the system do not develop during the simulation.

The leakance value may be physically based, representing the conductance associated with an aquifer between the model area and a large lake, or may be obtained through model calibration. The leakance value (C) for the scenarios illustrated in the preceding figure may be calculated using the following formula:

$$C = \frac{K \times L \times w}{M}$$

(10)

where:

 $L \times w$ is the surface area of the grid cell face exchanging flow with the external source/sink

K is the average hydraulic conductivity of the aquifer material separating the external source/sink from the model grid

D is the distance from the external source/sink to the model grid

When a General-Head boundary condition is assigned, the Use default leakance option is automatically selected.

If the "Use default leakance" option is selected, the General-Head boundary condition requires the following data:

- Stage: The head value for the external source/sink
- Leakance: A numerical parameter representing the resistance to flow between the boundary head and the model domain (this field is read-only and is calculated using formula described below)
- Distance to Reservoir. The distance from the external source/sink to the General-Head grid cell
- General Head Average Conductivity: The average hydraulic conductivity of the aquifer material separating the external source/sink from the model grid

The default formula used to calculate the Leakance value for the General-Head boundary is:

$$\$COND = \frac{\$KAVG \times \$FACEAREA \times \$UCTOCOND}{\$DIST}$$

(11)

where:

\$COND: is the Leakance for each General-Head grid cell

\$KAVG: is the Average Conductivity

\$FACEAREA: is the surface area of the selected grid cell Face for each General-Head grid cell (automatically calculated during translation)

\$UCTOCOND: is the conversion factor for converting the \$K value to the same Length (L) and Time (T) units used by \$COND. \$UCTOCOND is automatically calculated by Visual MODFLOW Flex.

\$DIST: is the Boundary Distance, the distance from the external source to the assigned general head boundary

If the "Use default conductance" formula option is not selected, the fields used for calculating the General-Head Conductance value (Distance to Reservoir, Average Conductivity) are removed from the table, and the Leakance field becomes a writable field where a value may be entered.

Supported Geometry

The geometry for General-Head boundary conditions can be specified using a polygon data objects.

Drain

VMOD Flex supports the standard Drain Boundary Package included with MODFLOW. The MODFLOW input data for Drain grid cells is stored in the projectname.DRN file. Currently, for finite element model translation, this boundary condition is not supported.

The Drain Package in MODFLOW is designed to simulate the effects of features such as agricultural drains, which remove water from the aquifer at a rate proportional to the difference between the head in the aquifer and some fixed head or elevation. The Drain package assumes the drain has no effect if the head in the aquifer falls below the fixed head of the drain.

Required Data

The Drain Package requires the following information as input for each cell containing this boundary condition:

- *Elevation*: The drain elevation, or drain head of the free surface of water within the drain. The drain is assumed to run only partially full, so that the head within the drain is approximately equal to the median elevation of the drain.
- Leakance: The drain leakance is a lumped coefficient describing the head loss between the drain and the groundwater system. This loss is caused by converging flow patterns near the drain, the presence of foreign material around the drain, channel bed

materials, the drain wall, and the degree to which the drain pipe openings may be blocked by chemical precipitates, plant roots, etc.

There is no general formulation for calculating drain leakance. In most situations, the detailed information required to calculate drain leakance is not available to the groundwater modeler. These details include the detailed head distribution around the drain, aquifer hydraulic conductivity near the drain, distribution of fill material, number and size of the drain pipe openings, the amount of clogging materials, and the hydraulic conductivity of clogging materials. It is common to calculate drain leakance from measured values of flow rate and head difference. Drain leakance value is usually adjusted during model calibration.

When a polyline is used to define the boundary condition geometry, the default formula for the leakance is as follows:

$$COND = RCHLNG \times LCOND$$
(11)

When a polygon is used to define the boundary condition geometry, the default leakance formula is as follows:

$$COND = DX \times DY \times SCOND$$

where:

\$COND: is the Leakance for each drain cell
\$RCHLNG: is the reach length of the drain in each grid cell
\$LCOND: is the Leakance per unit length of the drain in each grid cell
\$SCOND: is the Leakance per unit area of the drain in each grid cell
\$DX: is the length of each grid cell in the X-direction
\$DY: is the length of each grid cell in the Y-direction

If the Use default leakance option is turned off, the fields used for calculating the Drain Leakance value (Leakance per unit length or area) are removed from the table and the Leakance field becomes a read/write field where any value may be entered.

Supported Geometry

The geometry for General-Head boundary conditions can be specified using polygon or polylines

(12)

Streamflow-Routing (SFR2)

Flow in surface water systems is commonly more complex than the simple considerations included in the head-dependent flux boundaries such as RIV, DRN, and GHB packages described above. The streamflow-routing (SFR2) package was developed to include additional/optional complexities associated with surface water features, including:

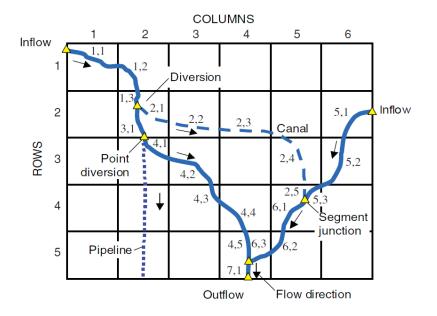
- mass balance (including optional flow routing) between stream reaches,
- · estimation of flow/water depth in stream reaches, and
- unsaturated flow to groundwater system from perched streams

For more information, see the USGS documentation for SFR1 (Prudic et. al., <u>2004</u>) and SFR2 (Niswonger and Prudic, <u>2005</u>). The <u>online documentation</u> for SFR2 contains additional information that supplements the USGS documentation, including documentation of the minor differences between the input structures for the versions of MODFLOW (e.g. - 2000, -2005, -NWT, -LGR).

Please note: SFR2 is not currently supported with MODFLOW-USG, MODFLOW-6, MODFLOW-SURFACT, or SEAWAT in Visual MODFLOW Flex.

Conceptualization in MODFLOW

Visual MODFLOW Flex supports surface water drainage systems as one or more networks of directed linear stream segments that may also be connected to polygonal lakes. Each segment or lake is an indexed single part polyline or polygon, respectively. The indices of each stream segment must ascend in the downstream direction and points of confluence (junctions) may either have multiple upstream connections to a single downstream segment (many to one) or one upstream connection to one or more downstream segments (one to many), but not multiple upstream connections to multiple downstream connections (many to many) as this configuration would lead to ambiguous flow routing given the algorithms implemented in SFR2.



Example Stream Network: streams are denoted by segment, reach. Where a segment is the polyline in the network and a reach is the portion of a segment within a given cell. Segment and reach indices must increase in the downstream direction.

Source: Prudic, et. al. (<u>2004</u>)

Mass Balance in Streams

Stream flows are estimated in the SFR2 package by a local and global mass balance on stream reaches within the network:

$$\sum [Q_{in}] - \sum [Q_{out}] = 0 \tag{13}$$

$$\left[Q_{sri} + \sum Q_{trb} + Q_{ro} + Q_{ppt} - Q_{gwl}\right] - \left[Q_{sro} + \sum Q_{div} + Q_{et} - Q_{gwu}\right] = 0$$
(14)

where:

 Q_{in} is the total inflow to a stream reach [L³/T]

 Q_{out} is the total outflow from a stream reach [L³/T]

 Q_{sri} is a specified inflow to the first reach in a segment [L³/T]. For segments originating within the model domain, this value is zero and non-zero for segments

at the model boundary with upstream flows from outside the lateral extents of the model,

 Q_{trb} is the estimated outflow from each upstream tributary [L³/T],

 Q_{ro} is the direct runoff from overland flow into the reach [L³/T],

 Q_{ppt} is the direct precipitation into the stream reach [L³/T],

 Q_{gwl} is the groundwater leakage from the stream reach to the hydraulically connected aquifer[L³/T]

 Q_{sro} is the estimated outflow from the reach [L³/T],

 Q_{div} is an optionally specified diversion from the reach [L³/T],

 Q_{et} is the direct evapotranspiration from the reach [L³/T],

 Q_{gwu} is the groundwater leakage from a perched stream reach to an underlying aquifer through the vadose zone [L³/T]

In order to estimate groundwater leakage from the stream (whether hydraulically connected or perched), the SFR2 package estimates the depth of the stream at the midpoint of each reach to obtain a head value by adding the estimated depth (d_{ri}) at the midpoint of the reach to the estimated bottom elevation of each reach (z_{ri}) . The bottom elevation at the midpoint is estimated by linearly interpolating the stream bottom elevations specified at the upstream and downstream ends of each segment.

Streamflow Diversions

In general, the stream network in the SFR2 package is assumed to bifurcate in the upstream direction only and the network always converges in the downstream direction towards a single watershed outlet. However, in some cases, flows in the downstream may diverge, either due to natural features (e.g. braided channels, sandbars, etc.) or constructed features (e.g. water intakes, irrigation ditches, canals, etc.). In the former case, where flow always converges, calculating the inflows to the downstream segment is trivial in that they are the sum of the outflows from the upstream segments. However, in the case where flows diverge in the downstream direction, the amount of flow must be divided up to each downstream segment. The SFR2 package provides four options:

- Reduce to available (IPRIOR=0): all available flow at the end of the last reach of a segment up to the rate specified will be diverted from the segment. Thus, if flow in the stream is less than the specified diversion, all available flow in the stream will be diverted, and none will remain in the channel. This option is common to many diversions in the western United States and is the default option for diversions.
- Reduce to None (IPRIOR=1): the specified diversion will only occur if flow in the stream is greater than that of the diversion, if flow is less than the specified diversion, then no flow is diverted and all flow remains in the channel.
- Fraction of Available (IPRIOR=2): a specified fraction of the available flow will be diverted

• Divert Excess (IPRIOR=3): all flow in excess of a specified rate will be diverted. This option is typically used for flood control in which all excess flow is diverted away from the main channel during peak discharge.

Water entering a diversion is subtracted from the end of the last reach of a segment; any remaining flow at the end of the last reach of a segment is added as tributary inflow at the beginning of the first reach in the next downstream segment.

Stream Depth

The depth of the stream in each reach is estimated using one of two supported options in Visual MODFLOW Flex:

- **Specified Depth (ICalc=0)**: the stream depth will be specified at both the upstream and downstream end of the segment and linearly interpolated to the midpoint of each reach
- Variable depth (ICalc=1): the stream depth will be estimated based on the estimated discharge at the midpoint of the stream and Manning's equation, as described below.

The estimated discharge at the midpoint of a reach is based on the assumption that the distributed inflows and outflows are uniform along the length of the channel, that point inflows are located at the upstream end of the reach, and that point outflows occur at the downstream end of the reach and are ignored as follows:

$$Q_{m} = Q_{sri} + \sum Q_{trb} + \frac{1}{2} \left(Q_{ro} + Q_{ppt} - Q_{et} - Q_{gwl} - Q_{gwu} \right)$$
(15)

The depth of the stream at the midpoint is estimated based on a rearranged form of the Manning equation for a "wide" rectangular channel (e.g. the stream is much wider than the depth of the stream and the hydraulic radius is approximately equal to the width of the stream):

$$d_m = \left(\frac{nQ_m}{CW\sqrt{S}}\right)^{3/5}$$

(16)

where:

 d_m is the estimated stream depth at the midpoint of the reach [L³/T],

n is the Manning roughness parameter [-],

C is a dimensional constant, which is 1.0 for flow units in m3/s and 1.486 for units of ft^3/s [L^{1/3}/T],

W is the width of the stream [-],

S is the slope of the reach which is estimated by Flex as from the segment length and its upstream and downstream elevations

In the case of variable stream depths calculated by the SFR2 package, the depth of the stream is both an input to the estimate of the groundwater leakance and is indirectly derived from it, which creates a circular dependence that is resolved using Newton-Raphson iterations and a specified tolerance as discussed in Prudic et al (2004).

Stream Leakance (Saturated)

In the case where the stream is directly connected to the groundwater system (i.e. the water table is above the bottom of the stream bed, stream leakance is calculated using the Darcy's law, similar to the implementation in the RIV package:

$$Q_{gwl} = \frac{AK}{m} \left(h_s - h_{gw} \right) \tag{17}$$

where:

A is (plan view) area of the streambed in the reach $[L^2]$,

K is hydraulic conductivity of the bed sediments [L/T],

m is the thickness of the bed sediments [L],

 h_s is the head in the stream reach [L],

 h_{gw} is the head in the groundwater system in the shared model cell [L].

In this case, the exchange between the groundwater system and the stream will be considered to occur instantaneously within the current time step.

Stream Leakance (Unsaturated)

The SFR2 package can also optionally include stream leakance through the unsaturated zone where stream reaches are perched (i.e. in cases where the calculated groundwater head in a cell falls below the bottom of the stream bed). In such reaches, the stream will discharge via the unsaturated zone using the same approach as implemented in the <u>UZF</u> <u>package</u> except:

$$Q_{gwl} = \frac{AK}{m} \left(h_s - z_b \right)$$

(18)

where:

 Z_b is the elevation of the stream bed [L]

Assumptions and Limitations

Major assumptions inherent in the SFR2 approach include the following:

- streamflow is one-dimensional and in the direction of the channel segments
- when the channel depth is specified as variable:
 - steady flow in the channel is assumed unless flow routing is active (i.e. TRANSROUTE is specified and IRTFLG=1), in which case the kinematic wave equation is used and dynamic wave effects are ignored
 - stream channels are sufficiently wide relative to stream depth such that the hydraulic radius is adequately described by the width of the stream in Manning's equation
 - a single value of Manning's roughness coefficient is adequate to estimate stream depths for the range of simulated discharges in each segment (e.g. the stream does not oscillate between flowing within the channel banks and spilling into the floodplain with a significantly different roughness)
 - o no backwater effects are considered
- flows are routed to downstream reaches based on continuity and the SFR package is not recommended for modeling the surface water flows, depths, or the transient exchange of water between stream reaches and the groundwater system for evaluations of short-term (seconds to days) effects. The inclusion of the kinematic wave routing (i.e. TRANSROUTE option and IRTFLG=1) may provide some improvements as described in Markstrom, *et al.* (2008).

Other assumptions are also inherent in the implementation of SFR2, a more comprehensive complete list of the assumptions is included in the documentation references discussed above which should be consulted as part of the model development process.

Required Parameters

In Visual MODFLOW Flex, the SFR2 Package requires a more complex set of inputs than the other boundary conditions and as such is defined in its own <u>workflow</u>. Surface Water inputs are grid independent and are based on a set of parameterized vector geometries that define the surface water network consisting of connected/directed stream segments and optional lake polygons. Inputs for each of these is defined in the <u>Surface Water Network</u> <u>Data</u> section.

Supported Geometry

Surface Water inputs are grid-independent and are based on a set of parameterized vector geometries that define the surface water network consisting of connected/directed stream segment polylines and optional lake polygons. A more complete description can be found in the <u>surface water workflow</u> description.

Recharge

Visual MODFLOW Flex supports the Recharge Package (RCH) included with MODFLOW. The Recharge input data for MODFLOW is stored in the projectname.RCH file. For finite element models, recharge boundary conditions are translated as the In(+)/Out(-)flow material parameter.

The recharge boundary condition is typically used to simulate surficially distributed recharge to the groundwater system. Most commonly, recharge occurs as a result of precipitation percolating into the groundwater system. However, the recharge boundary can potentially be used to simulate recharge from sources other than precipitation, such as irrigation, artificial recharge, or seepage from a pond.

Please Note: The recharge rate is a parameter that is not often directly measured at a site, but rather, it is often assumed to be a percentage of the precipitation. This percentage typically ranges from 5% to 20% of total precipitation depending on many different factors including the predominant land use and vegetation type, the surface topography (slope), and the soil cover material

Required Data

The Recharge Package requires the following information as input for each cell containing this boundary condition:

- Recharge (L/T): The input flux due to recharge. The recharge is applied in one of three ways as part of the package translation settings: 1. recharge is applied only to cells in layer 1, 2. recharge is applied to cells the specified layer, 3. recharge is applied to the upper-most active cell. See the documentation in the <u>Recharge Translation</u> <u>Settings</u> documentation for more details.
- Ponding (L) [optional, only used in the MODFLOW-SURFACT engine]: The maximum allowable depth of the water table above the ground surface. Calculated heads elevations above this depth (+ground surface) are truncated by the model.

Please Note: MODFLOW-SURFACT simply removes excess ponded water from the model without routing it to other cells.

Supported Geometry

The geometry for Recharge boundary conditions can be specified using polygon data objects and by points, and for an entire layer.

Evapotranspiration

Visual MODFLOW Flex supports the Evapotranspiration Package (ET) included with MODFLOW. After translation, the Evapotranspiration input data for MODFLOW is stored in the projectname.EVT file. Currently, this boundary condition is not supported for finite element translation.

The evapotranspiration boundary condition simulates the effects of plant transpiration, direct evaporation, and seepage at the ground surface by removing water from the saturated groundwater regime.

The evapotranspiration boundary approach is based on the following assumptions:

- When the water table is at or above the ground surface (top of layer 1), evapotranspiration loss from the water table occurs at the maximum rate specified by the user.
- When the elevation of the water table is below the 'extinction depth', or is beneath layer 1, evapotranspiration from the water table is negligible.

Between these limits, evapotranspiration from the water table varies linearly with water table elevation.

Required Data

The Evapotranspiration Package requires the following information:

- Evapotranspiration rate: The rate of evapotranspiration as it occurs when the water table elevation is equal to the top of the grid cell elevation. This value should be entered in the units set for recharge as defined in the Project Settings.
- Extinction Depth: The depth below the top of grid cell elevation where the evapotranspiration rate is negligible.

The Evapotranspiration Package approach is based on the following assumptions:

- When the water table is at or above the ground surface (top of layer 1), evapotranspiration loss from the water table occurs at the maximum rate specified by the user.
- When the elevation of the water table is below the 'extinction depth' relative to the top of the model, evapotranspiration from the water table is negligible (i.e. set to zero).

Evapotranspiration from the water table varies linearly with water table elevation between these limits.

Supported Geometry

The geometry for Evapotranspiration boundary conditions can be specified using polygon data objects

Lake

Visual MODFLOW Flex supports the Lake (LAK3) package for MODFLOW. After translation, the Lake input data for MODFLOW is stored in the projectname.LAK file.

The lake boundary condition can be used to simulate the effects of stationary surface-water bodies such as lakes and reservoirs on an aquifer. The lake boundary is an alternative to the traditional approach of using the general head boundary condition. The main difference in the lake boundary is that the lake stage is calculated automatically based on the water budget, which is a function of inflow, outflow, recharge, etc.

For more information on the Lake package, please refer to Merritt and Konikow (2000).

Required Data

The lake package requires the following input parameters:

- Stage [L]: The initial stage of the lake at the beginning of the run.
- *Bottom [L]*: The elevation of the bottom of the seepage layer (bedding material) of the surface water body.
- Leakance [L²/T]: A numerical parameter representing the resistance to flow between the boundary head and the model domain (this field is read-only and is calculated using formula described below)
- Lakebed Thickness [L]: Thickness of the lakebed (seepage layer).
- Lakebed Conductivity [L]: Vertical hydraulic conductivity of the lakebed material.
- *Precipitation Rate per Unit Area [L/T]*: The rate of precipitation per unit area at the surface of the lake.
- Evaporation Rate per Unit Area [L/T]: The rate of evaporation per unit area from the surface of the lake.
- Overland Runoff [L³/T]: Overland runoff rate from an adjacent watershed entering the lake.
- Artificial Withdrawal [L³/T]: The volumetric rate of water removal from a lake by means other than rainfall, evaporation, surface outflow, or ground-water seepage. Normally, this would be used to specify the rate of artificial withdrawal from a lake for human water use, or if negative, artificial augmentation of a lake volume for esthetic or recreational purposes.

The default leakance formula is as follows:

$$\$COND = \frac{\$DX \times \$DY \times \$K \times \$UCTOCOND}{\$RBTHICK}$$

(20)

where:

\$COND: is the Conductance

\$K: is the vertical hydraulic conductivity of the lakebed

\$UCTOCOND: is the conversion factor for converting the \$K value to the same L and T units used by \$COND. \$UCTOCOND is automatically calculated by Visual MODFLOW Flex.

\$RBTHICK: is the Lakebed Thickness

\$DX: is the length of each grid cell in the X-direction

\$DY: is the length of each grid cell in the Y-direction

If the "Use default Leakance" option is turned off, the fields used for calculating the River Conductance value (Lakebed Thickness, Lakebed Kz) are removed from the table, and the Leakance field becomes a writable field where a value may be entered.

Supported Geometry

The geometry for Lake boundary conditions can be specified using polygon data objects.

Specified Flux

When you create the flux object, the value you define should be the flux per unit length (when using polyline) or per unit area (for polygon). When the cell realization is calculated, then VMOD Flex will calculate the flux for each cell based on the length of the line that passes thru the cell (for polyline) or the cell area (for polygon). For these reasons, you will see a significant difference in the parameter values for the conceptual object (shape) vs. the summed values for all cells (the cell realization).

VMOD Flex supports the Specified Flux (FHB1) package for MODFLOW. After translation, the specified flux input data for MODFLOW is stored in the projectname.FHB file. Currently, translation of this boundary condition is not supported for finite element models.

The Specified Flux boundary condition allows you to specify flow, as a function of time, at selected model cells. FHB1 is an alternative and (or) supplement to the recharge (RCH) package for simulating specified-flow boundary conditions. The main differences between the FHB1 package and the recharge package are as follows:

- FHB1 package can simulate specified-flux on the top, side, bottom or intermediate layers in the simulation domain, whereas the recharge package can only be applied to the top and intermediate layers.
- FHB1 package allows you to specify a starting flux and an ending flux (for each stress period, if transient). The package then uses linear interpolation to compute values of flow at each model time step.

For more information on the Specified-Flow (FHB1) package, please refer to Leake and Lilly (<u>1997</u>).

Required Data

The specified flux package requires the following input parameters:

- Starting Flux (L³/T)
- Ending Flux (L³/T)

Supported Geometry

The geometry for Specified Flux boundary conditions can be specified using polygon or polyline data objects.

Time-Varying Material Properties

Time-varying material properties can be specified for transient groundwater flow simulations (using the TMP1 package add-on in MODFLOW-SURFACT). The list of time-dependent properties includes:

- horizontal hydraulic conductivity,
- either vertical hydraulic conductivity or leakance,
- specific storage, and
- specific yield.

The reference values of these properties are assigned in the standard format associated with the BCF4 package. These reference values are then scaled by factors assigned in the TMP1 package, where the factors are time-dependent over the simulation period.

Required Data

The time-varying material package requires the following dimensionless input parameters for each stress period specified in the boundary condition:

- **Kxx/Kyy Scaling** [-]: the scaling factor by which the base horizontal conductivities (Kxx and Kyy) values will be multiplied for the associated stress period
- **Kzz Scaling** [-]: the scaling factor by which the base vertical conductivity (Kzz) value will be multiplied for the associated stress period
- Leakance Scaling [-]: the scaling factor by which the base vertical leakance values will be multiplied for the associated stress period.
- Sy Scaling [-]: the scaling factor by which the base specific yield values will be multiplied for the associated stress period.
- **Ss Scaling** [-]: the scaling factor by which the base specific storage values will be multiplied for the associated stress period.

Please Note: the Kzz and Leakance Scaling factors are mutually exclusive and which one is used is based on the settings in the BCF4 package.

Supported Geometry

The geometry for time-varying material boundary conditions can be specified using polygon or polyline data objects or on a cell-by-cell basis.

Unsaturated Zone Flow (UZF)

Visual MODFLOW Flex supports estimations of flow through the unsaturated zone using the Unsaturated Zone Flow (UZF) package included with most versions of MODFLOW. The UZF input data for MODFLOW is stored in the projectname.UZF file.

Conceptualization in MODFLOW

The UZF boundary condition is typically used to simulate distributed recharge and evapotranspiration to and from the groundwater system through the vadose zone.

<u>Recharge</u>

The recharge rate through the vadose zone is estimated using a vertical 1-D kinematic wave approximation of the Richard's equation and some simplifying assumptions as described by Niswonger et al. (2006) to estimate flow at a sharp front wetting front advancing at a velocity:

$$q_f = \frac{K(\theta_1) - K(\theta_2)}{\theta_1 - \theta_2}$$

where:

 q_f is the velocity of the sharp wetting front [L/T],

 θ_1 is the water content above the wetting front [-],

 $heta_2$ is the water content below the wetting front [-],

 $K(\theta_1)$ is the hydraulic conductivity above the wetting front given θ_1 [L/T], and

 $K(\theta_2)$ is the hydraulic conductivity above the wetting front given θ_2 [L/T]

The hydraulic conductivity is related to the water content based on the Brooks-Corey relationship:

$$K(\theta) = K_{sat} \left[\frac{\theta - \theta_r}{\theta_s - \theta_r} \right]^c$$
(22)

where:

 K_{sat} is the saturated vertical hydraulic conductivity of the vadose zone [L/T],

 θ is the water content [-],

 θ_r is the residual water content [-],

 θ_s is the saturated water content [-], and

 ε is the Brooks-Corey exponent [-]

The recharge rate at the infiltration boundary (q_{in}) is specified and the corresponding water content is estimated using the following equation:

(21)

$$\theta = s_{\mathcal{Y}} \left(\frac{q_{in}}{K_{sat}} \right)^{1/\varepsilon} + \theta_r, \left[0 < q_{in} \le K_{sat} \right]$$
(23)

$$=\theta_{s}\left[K_{sat} < q_{in}\right] \tag{24}$$

where:

θ

 S_{y} is specific yield of water table aquifer [-]

Evapotranspiration

Evapotranspiration, the combined effect of direct evaporation and uptake by plant roots in the unsaturated zone, is a process that causes water to move upward from the base of the root zone to the surface. The rate of evaporation in the unsaturated zone is estimated in the UZF package based on the same principles as in the <u>EVT package</u> with the exception that evapotranspiration is also to zero when the water content in the vadose zone is less than the extinction water content.

Material Properties

The UZF package also includes static parameters to define the material properties of the unsaturated zone, including the Brooks-Corey exponent (ϵ), saturated water content, and initial water content. Note that the residual water content is assumed to be the specific yield. For more information, please refer to the discussion on the <u>vadose zone properties</u>.

Required Data

The Recharge Package requires the following information as input for each cell containing this boundary condition:

- Infiltration Rate [FINF]: The potential input flux due to recharge [L/T]
- Potential Evapotranspiration Rate [PET]: The potential evapotranspiration rate [L/T]
- Extinction Depth [EXTDP]: The depth at which PET decreases linearly to zero [L]
- Extinction water Content [EXTWC]: the water content below which evapotranspiration ceases [-]. (θ_s) ≤ EXTWC ≤ (θ_s − S_y)

Supported Geometry

The geometry for UZF boundary conditions can be specified using polygon data objects, by points, or for an entire layer.

Mass Source Loading (SRC) - Specified Mass Flux)

When you create the mass source loading object (which consists of a specified mass flux), the value you define should be the mass flux per unit length (when using polyline) or per unit area (for polygon). When the cell realization is calculated, then VMOD Flex will calculate the flux for each cell based on the length of the line that passes thru the cell (for polyline) or the cell area (for polygon). For these reasons, you will see a significant difference in the parameter values for the conceptual object (shape) vs. the summed values for all cells (the cell realization).

VMOD Flex supports the Flux (SRC) package for MODFLOW-6 models only. After translation, the specified flux input data for MODFLOW is stored in the . \GWT\S###\projectname.SRC file, where ### is the index of the species.

The Mass Source loading boundary condition allows you to specify flux as a function of time, at selected model cells. For more information on the

Required Data

The specified flux package requires the following input parameters:

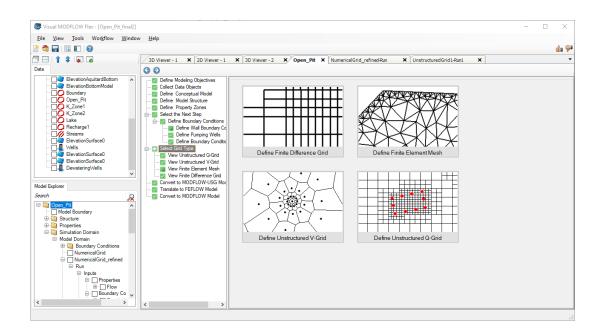
Mass Flux (M/(TL) for polylines, M/(TL²) for polygons, and M/T for cells

Supported Geometry

The geometry for conceptual Mass Source Loading boundary conditions can be specified using polygon or polyline data objects.

8 Defining Grids/Meshes

At this step, you can create finite difference grids for MODFLOW, unstructured grids for MODFLOW-USG, or finite element meshes for a FEFLOW run.



Quick Overview

Instructions	 Define Finite Difference Grid; Define UnStructured Grid;
	 <u>Define Finite Element Mesh</u>
Pre-requisites:	The Conceptual Model has been defined.
Result:	A numerical grid or mesh is created.
Next Steps:	Convert the conceptual model to any one
	of the following:
	 <u>Convert to a MODFLOW (finite</u>
	difference) model;
	 <u>Convert to a MODFLOW-USG model</u>
	Convert to a FEFLOW finite element
	model

Once you have created your conceptual model you can discretize your model using either the finite difference method, unstructured finite volume (Control Volume Finite Difference, CVFD) or the finite element method. The finite difference method involves fitting your

conceptual model to one or more finite difference grids. The CVFD method (used in MODFLOW-USG), allows you to conform the grid to your wells and boundary conditions. For MODFLOW-based numerical models, after conversion, the resulting numerical model can be viewed/edited and then simulated in the Visual MODFLOW Flex environment. The finite element method involves fitting your conceptual model to a finite element mesh. Once translated, a FEFLOW ASCII .FEM file is created (and saved on the hard disk), which can then be opened and simulated using FEFLOW.

Please Note: a license of FEFLOW v.5.4 or above is required to open FEFLOW .FEM files generated from Visual MODFLOW Flex.

Sections covered in this chapter:

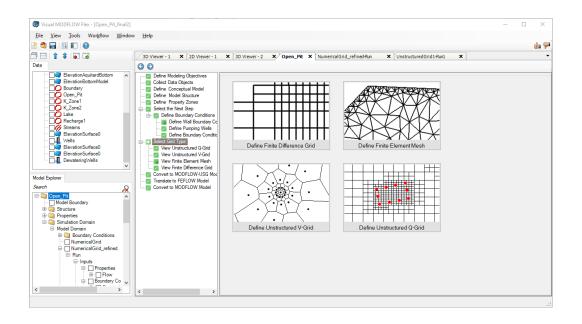
- Define Finite Difference Grid
- Define UnStructured Voronoi Grid (V-Grid)
- Define Unstructured Quadtree Grid (Q-Grid)
- Define Finite Element Mesh

8.1 Define Finite Difference Grid

Quick Overview

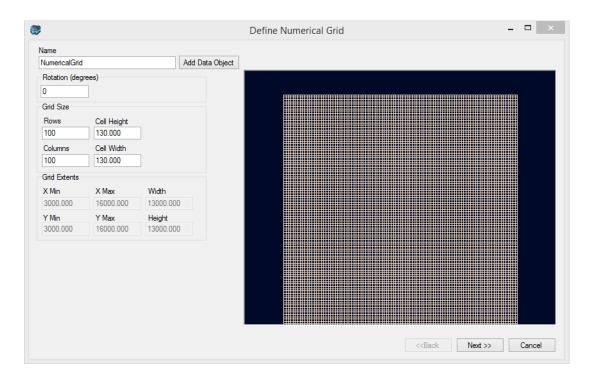
Instructions	Specify the horizontal grid resolution and the vertical layering type and resolution
Pre-requisites:	The Conceptual Model has been defined.
Result:	A numerical grid is created
Next Steps:	Convert the conceptual model to a
	MODFLOW model

From the "Select Grid Type" step in the Conceptual Model workflow, click on the "Define Finite Difference Grid button":



Defining the Horizontal Grid

By default, Visual MODFLOW Flex discretizes the horizontal grid using 20 rows and 20 columns, with no rotation. However, you can customize the grid to your liking, by modifying the settings in the horizontal grid dialog (shown below).



• Enter a unique Name for the numerical grid. This name will appear in the Model Explorer tree once the grid is created.

- The grid can be rotated counter-clockwise about the grid origin by entering a value between 0 and 360 in the Rotation text field.
- The Xmin and Ymin values refer to the X-Y coordinates of the bottom-left corner of the numerical grid. The Xmax and Ymax values refer to the X-Y coordinates of the top-right corner of the numerical grid.
- The Columns and Rows fields allow you to define the Grid Size.
- You can also specify the Cell Height and Cell width and the Rows and Columns (and potentially the extents) will be updated accordingly.
- Click the [Next] button to proceed to define the vertical discretization.

Defining the Vertical Grid

The first step in defining the vertical grid is selecting the Grid Type.

#		Define Numerical Grid – 🗖 🗙
layers follow the horizons e layers, by dividing the zone Min Cell Thickness 0.1	Create Child Grid Create Child Grid the tops and bottoms of the model evations. You can refine the model es into proportionately thick layers. Zmin 184.524382230466 Zmax 367.417941186982	
Layer Name Zone1 Zone2	Layer Refinement 1 1	
	Apply	Exaggeration 40 🐑 Row 1 🐑 Column 1 🗘

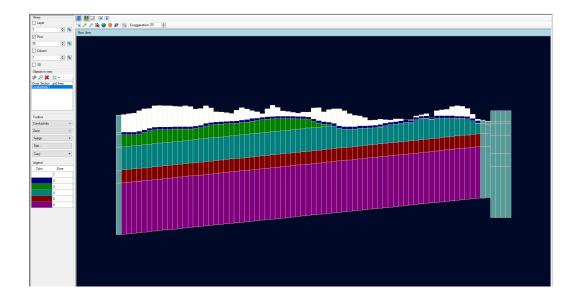
Grid Types

There are three different grid types: Deformed, Uniform and Deformed-Uniform. Each grid type is described in the following sections.

Deformed

In a deformed grid, the tops and bottoms of the model layers conform to the horizon elevations. You can refine the model layers, by diving the structural zones into proportionately thick layers.

Cross sectional view of a deformed grid from Visual MODFLOW Flex



A Minimum Cell Thickness must be specified as MODFLOW does not permit lateral discontinuity of layers, i.e., a layer cannot have a thickness of 0 at any point in the layer. When horizons are on-lapping one another, resulting in a zero cell thickness, the minimum cell thickness is applied and the horizons are shifted based on the horizon types defined in the Horizon settings (See "Horizon Types" section).

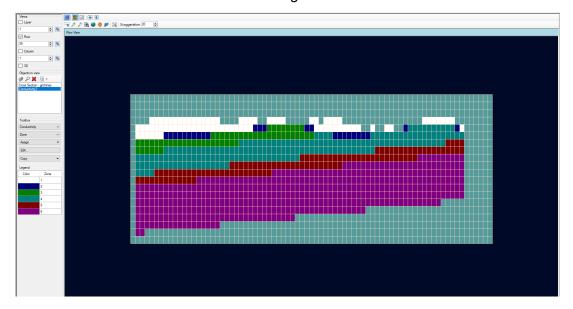
For deformed grids, you have the option of refining (subdividing) each layer into a specified number of equally thick layers. In the table located below the grid description, enter a refinement factor for the desired layer(s). For example, a layer refinement factor of 2 would subdivide the layer into two equally spaced layers.

Layer Name	Layer Refinement
Zone1	2
Zone2	2
Zone3	1

After entering a refinement factor, click the [Apply] button to view the changes in the adjacent 2D Viewer.

Uniform

In a uniform grid, a number of layers with uniform thickness will be created. At the time of translating the conceptual model to the numerical model, the properties will be assigned to the appropriate grid cells to represent the geological structure. This grid is useful for transport or density-dependent simulations, where it is desirable to have fine vertical discretization.



Cross sectional view of a uniform grid from Visual MODFLOW Flex

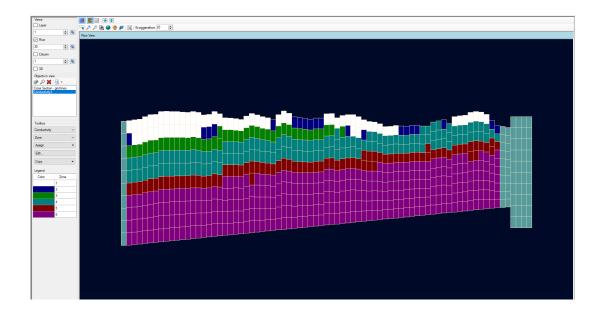
When this grid type is selected, specify the number of layers to create in the Number of Layers field (default is 10).

Please Note: Maximum number of vertical layers is 1000.

Semi-Uniform

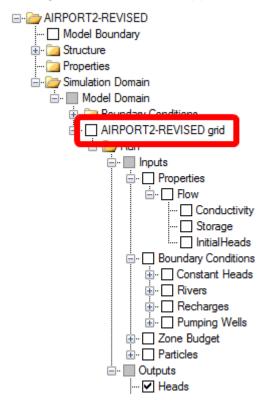
In a semi-uniform grid, the top and bottom of the grid are deformed, following the top-most and bottom-most horizons respectively; in between, a set of uniformly thick layers will be generated. At the time of translating the conceptual model to the numerical model, the properties will be assigned to the appropriate grid cells to represent the geological structure. This grid is useful where you have discontinuous layers.

Cross sectional view of a semi-uniform grid from Visual MODFLOW Flex



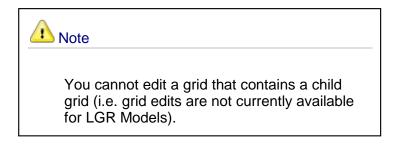
For Deformed-Uniform grids, you must specify a Minimum Cell Thickness (see above) and the Number of Layers.

Once the grid is created, it will appear as a new node in the tree as shown below:



8.1.1 Edit Grid

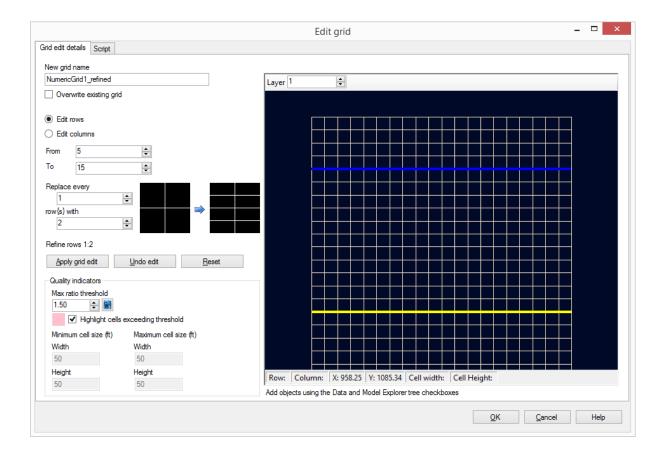
When a numerical grid is initially created (see "<u>Creating a Finite Difference Grid</u>" section), the horizontal grid spacing is uniform. However, in many situations it is advantageous to have non-uniform grid spacing to allow for finer grid discretization in the areas of interest, and larger grid spacing in areas which are less important, or where less data is available. Visual MODFLOW Flex allows you to refine or coarsen areas of a numerical grid by adding or removing grid lines within a specified row/column interval. This process is described in the following section.



To edit the grid (rows and columns) select the View/Edit Grid step of the Numerical Workflow and then select the Edit grid button. Alternatively, you can find this option from the Model Explorer tree, right-click on the Numerical Grid, and select Edit Numerical Grid from the popup menu.

The Edit grid dialog provides options for refining/coarsening a numerical grid.

When you edit the grid by default you are creating a new grid - and a default New grid name is generated (you can adjust this if you wish). If however, you prefer to simply overwrite your existing grid with the changes you make simply select the check box to do so.



Tip! You can add data objects (e.g., boundary conditions, wells, site maps) from the data explorer to the 2D Viewer preview to assist you in determining the areas in which horizontal refinement/coarsening should be applied. Select the desired data objects from the Data Explorer, and the data will be displayed in the 2D Viewer preview.

- Select the Edit Rows radio button to add/remove grid lines (rows) along the Y-direction of the numerical grid, or select the Edit columns radio button to add/remove grid lines (columns) along the X-direction of the numerical grid.
- Specify the row/column interval for which the refinement/coarsening should be applied, by specifying the From row/column and the To row/column. For example, if you would like to refine the grid area between row 20 and 30, you would enter 20 as the From row and 30 as the To row. In the preview the blue line represents the From row/column while the yellow line represents the To row/column.
- Next, specify the refinement/coarsening factor. In the example above we are going to Replace every 1 row with 2 so the grid will be refined. This means that we would subdivide each row within the specified interval into two equally spaced rows.

- Instead, if we changed the option to indicate we are going to Replace every 2 rows with 1 then the grid would be coarsened. This means we would reduce the number of rows within the specified interval by a factor of 2.
- When you select the Apply grid edit button the preview will be updated with your edits. You also have options to Undo your edit - this will undo your last change. You can keep selecting Undo edit to undo more changes. Reset will return the preview to the original rows and columns.
- Click the OK button to create the new refined/coarsened grid. You will find it in the Model Explorer.

When editing a grid all inputs from the original grid (property zones, boundary conditions, pumping wells, observation wells, zone budget zones, and particles) will be reassigned as appropriate to the new edited grid. If the original grid has multiple runs associated with it - the inputs are taken from the first run.

Quality Indicators

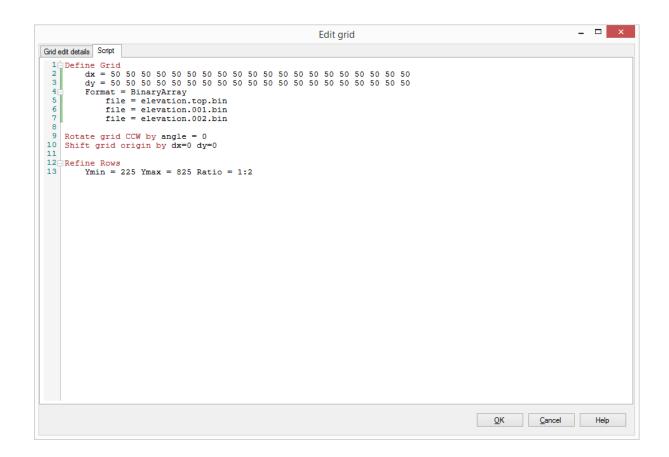
The quality indicators can help you find areas in your grid where you may wish to make adjustments. By default the Maximum ratio threshold is 1.5 however you can adjust this to your model requirements. If you do not wish to have the Quality indicators on simply uncheck the Highlight cells exceeding threshold option.

Also displayed in the Minimum and Maximum cell size.

Max ratio threshold				
1.55 🖨 😹				
Highlight cells exceeding threshold				
Maximum cell size (ft)				
Width				
50				
Height				
50				
,	Maximum cell size (ft) Width 50 Height			

Script

If preferred, you can make your grid edits by using the Script option. On this tab you will find the script for any edits you make on the Grid edit details tab allowing you to learn the script language.



8.1.2 Edit Layers

To edit the grid (layers) select the View/Edit Grid step of the Numerical Workflow and then select the Edit layers button. Alternatively, you can find this option from the Model Explorer tree, right-click on the Numerical Grid, and select Edit Grid Layers from the pop-up menu.

The Edit layers dialog provides options for refining/coarsening/editing a numerical grid. When you edit the grid by default you are creating a new grid - and a default New grid name is generated (you can adjust this if you wish at the time the new grid is generated - once a grid is created, it cannot be renamed). If however, you prefer to simply overwrite your existing grid with the changes you make, simply select the check box to do so.

The dialog also provides you with a preview of the grid layers as viewed by a Row or a Column - you can select this from the Viewing drop down options above the preview window. You can then adjust which Row or Column you are viewing using the up and down arrows as well as the Exaggeration.

When you select the Apply edit button the preview will be updated with your edits. You also have options to Undo your edit - this will undo your last change. You can keep selecting Undo edit to undo more changes. Reset will return the preview to the original rows and columns.



You can add data objects (e.g., boundary conditions, wells, etc.) from the data explorer to the preview to assist you in determining the areas in which refinement/coarsening should be applied. Select the desired data objects from the Data Explorer, and the data will be displayed in the preview.

Edit Layers Dialog

The Edit Layers dialog provides several options for adjusting the layers of your model, including:

- Refine: subdivide one or more model layers by a (whole number) factor,
- Insert: subdivide a model layer by inserting a new surface into the model
- <u>Remove</u>: coarsen the model by removing a surface from the model
- <u>Replace</u>, adjust the elevation of a model layer by replacing the top (or bottom) elevations of a model layer
- Cells: adjust the elevations of individual cells
- <u>Script</u>: use a script to define the elevation of individual cells

These options are described in detail below.

Creating New Grids - Applying and Committing Edits to Grid Layers

To implement or preview any of the edits described below, first click the **Apply edit** button, you can where you can review and inspect the changes. You must click the Apply edit button for each individual change to the grid. Applied edit(s) to the grid layers will be saved into a new grid with the name entered under the **New grid name** option once you click the **OK** button. If you may choose to **overwrite the existing grid**, in which case the edited grid will replace the existing grid. If the current grid is associated with more than one model run (e.g. you have cloned one or more models associated with the grid or created updated run(s) using PEST, etc.) then you will be prompted to select which runs should be included with the updated/new grid layers.

Edit layers Layer edit details Script	– 🗆 X
New grid name NumericalGrid_refined Overwrite existing grid Refine Insert Remove Replace Cells From layer 2 To layer 5 By a factor of 2	Viewing Row 35 (2) Exaggeration 20 (2) (2) (2) (2) (2) (2) (2) (2) (2) (2)
Apply edit Undo edit Reset	Add objects using the Data and Model Explorer tree checkboxes
	OK Cancel Help

Minimum Layer Thickness

Some layer editing options (i.e. <u>insert</u> and <u>replace</u>) include settings to ensure that edits to grid layer do not result in layers with thicknesses below a specified threshold (i.e. **the minimum layer thickness**) – this is an important consideration in grid design as models with overly thin model cells may result in numerical instabilities and convergence issues.

The default **minimum layer thickness** in Visual MODFLOW Flex is 0.1 measurement units (i.e. feet or meters).

Refine Insert Remove Replace Cells	Refine Insert Remove Replace Cells
Fraction of layer Thickness below layer ceiling Push down Thickness below layer ceiling	Top of layer Bottom of layer Push down
 Thickness above layer floor At elevation Layer 4 Fraction 0.01 	1 Image: Constraint of the second s
Minimum layer thickness 0.10 🚖 m	1.00 m Minimum layer thickness 0.10

The **Push up** and **Push down** options are provided to determine how layers should be adjusted (if necessary) to so that resulting layers are not thinner than the specified threshold:

• When <u>neither</u> Push up nor Push down are selected, then the new surface (or applicable portions of the new surface) will be raised above existing surfaces below the insertion point and the new surface (or applicable portions of the new surface) will be lowered below existing surfaces above the insertion point such that the minimum layer

thickness criteria is obeyed. In this case, only (applicable portions of) the new surface will be adjusted to to enforce the minimum layer thickness criteria. If the elevation difference between the surfaces immediately above and below the new surface (or portions thereof) is less than twice the minimum thickness, the minimum layer thickness criteria will not be satisfied and you will be prompted with a warning message.

- When only <u>Push up</u> is selected, then applicable surfaces (or applicable portions of surface) above the new surface will be sequentially raised (pushed up) above this new surface such that the Minimum layer thickness criteria is obeyed. In this case, the layer below the new layer may push the new layer itself upwards and this push may propagate upwards through the model layers to enforce the minimum layer thickness criteria.
- When only <u>Push up</u> is selected, then applicable surfaces (or applicable portions of surface) above the new surface will be sequentially raised (pushed up) above this new surface such that the Minimum layer thickness criteria is obeyed. In this case, the layer above the new layer may push the new layer itself downwards and this push may propagate downwards through the model layers to enforce the minimum layer thickness criteria.
- When <u>both Push up and Push down</u> are selected, then the new surface will combine the individual behavior of when Push up or Push down are selected - that is, the new surface will push (applicable portions of) surfaces above and below away from the new surface such that the minimum layer thickness criteria is obeyed. In this case, all layer adjustments would propagate outwards from the new layer and (applicable portions of) layers above and below the new layer may be adjusted to enforce the minimum layer thickness criteria.

Refine

You can select the **from layer** and **to layer** values and then provide a **Factor** to refine by. For example if you have 6 model layers and indicate the From 3 To 5 and a factor of 2 (as shown below) when you select the Apply edit button, you would end up with a total of 9 layers (as three of the original layers would remain unchanged and three of the layers would be split into 2).

Edit layers Layer edit details Script New grid name	- D X
NumericalGrid_refined	Viewing Row 🔹 35 🚖 Exaggeration 20 🚖 🔎 🔎 🏠 🌺
Overwrite existing grid	
Refine Insert Remove Replace Cells From layer 2 - - To layer - - 5 - - By a factor of 2 -	Layer: 1 Row: 1 Column: 1 X: -848.81 Z: 246.05
Apply edit Undo edit Reset	Add objects using the Data and Model Explorer tree checkboxes
	OK Cancel Help

Insert

You can select to insert a new layer using the following options:

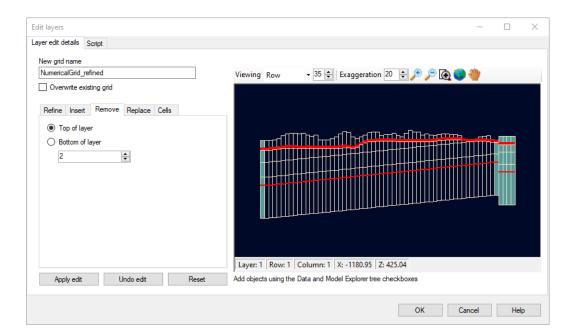
- Fraction of layer
- Thickness below layer ceiling
- Thickness above layer floor
- At elevation

When you select which option you want to use you will see in the preview that the selected layer is highlighted in green and when you hover your mouse over the preview the proposed new layer to be inserted will appear as a red line. You can also click on the grid to select where to place the inserted layer using the selected option (e.g. fraction, thickness, or constant elevation).

	id_refined			Viewing Row	▪ 35 🚔 Exagg	jeration 20 🚔 🍠) 🔎 🙆 🤍	-	
Refine In Fracti Thick Thick At ele Layer 4 Fracti 0.01	on of layer ness below laye ness above laye vation	er floor •							
Apply e	dia	Undo edit	Reset	Add objects using the	Column: 1 X: -129				

Remove

On this tab you can simply select the layer you wish to remove from the preview window using the mouse or you can specify whether the Top or Bottom of the indicated layer is to be removed.



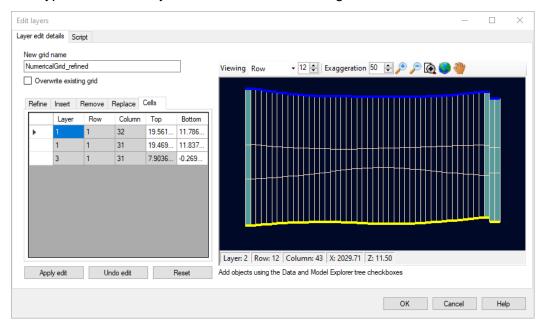
Replace

This tab provides the option to replace either the top or the bottom of a layer with an existing surface (selected from the Data Explorer and using the add button) or at a specified elevation.

Edit layers Layer edit details Script New grid name NumericalGrid_refined Overwrite existing grid	- □ × Viewing Row • 35 € Exaggeration 20 € ♪ ♪ [@ ● 🁋
Refine Insert Remove Replace Cells Top of layer Push up Bottom of layer Push down 1 Use surface object New surface name Use elevation 1.00 m Minimum layer thickness 0.10 m Apply edit Undo edit Reset	Layer: 1 Row: 1 Column: 1 X: -1180.95 Z: 425.04
	OK Cancel Help

Cells

This tab provides allows you to make specific edits to a small number of cells. Use the view settings to find the desired cells in a Row or Column view and click on the cell(s) to be edited. Type in the values you wish to use in the new grid.



Script

If preferred, you can also make your layer edits by using the Script option. On this tab, you will find the script for any edits you have applied on the Layer edit details tabs allowing you to learn the script language. By making a few changes in the Layer edit details tab (i.e. the options discussed above), you can easily discover the relatively simple syntax of the script. An example of edits to cells and minimum layer thickness settings are shown below. In this manner, advanced users can rapidly incorporate changes to grid layers using external tools such as spreadsheets or custom codes with minimal additional effort:

```
Edit layers
                                                                                                                                    \times
Layer edit details Script
 1-Define Grid
          = BinaryArray
          Format
              file = elevation.top.bin
file = elevation.001.bin
 6
              file = elevation.002.bin
file = elevation.003.bin
file = elevation.003.bin
10 Rotate grid CCW by angle = 0
11 Shift grid origin by dx=19.742 dy=0
13 Modify Surface Index = 0 Min Thickness = 0.1 Push Down = False Push Up = False
            32 19.5612644304365
31 19.4692083651843
       1
15
13 13 19.5092053051843
16.Modify Surface Index = 1 Min Thickness = 0.1 Push Down = False Push Up = False
17 1 32 11.7866962682729
18 1 31 11.837544711269
19 Modify Surface Index = 3 Min Thickness = 0.1 Push Down = False Push Up = False
20
              31 -0.269808602472649
21
<
                                                                                                  OK Cancel Help
```

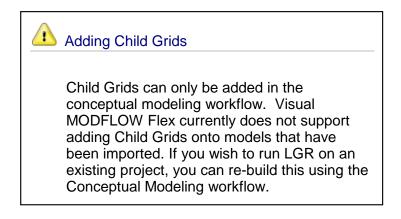
8.1.3 Define Child Grid (for LGR)

A higher-resolution block-shaped child grid can be created within any numerical grid (parent grid) and used for running Local Grid Refinement (LGR) simulations with the MODFLOW-2005 LGR package. Refined child grids are often used to improve simulation accuracy around areas of interest within your simulation domain. For example, refined grids may be needed in:

- Regions where hydraulic gradients change substantially over short distances, as would be common near pumping or injecting wells, rivers, drains, and focused recharge.
- Regions of site-scale contamination within a regional aquifer where simulations of plume movement are of interest.

 Regions requiring detailed representation of heterogeneity, as may be required to simulate faults, lithologic displacements caused by faulting, fractures, thin lenses, pinch outs of geologic units, and so on.

Visual MODFLOW Flex allows you to create up to nine child grids within a single parent grid. However, you cannot create a child grid within a child grid, and child grids cannot not overlap and must have at least one parent grid cell in between them.



For more information on the local grid refinement package, please refer to the <u>online guide</u> for MODFLOW-LGR and to the published documentation by Mehl and Hill (<u>2005</u>, <u>2013</u>).

There are two ways in which you can define a child grid within a numerical model grid:

- When defining the parent grid; check the Create Child Grid box in the Vertical Grid dialog, and click the [Next] button.
- After the parent grid has been defined; right-click on the numerical grid from the Model Explorer tree, and select Create Child Grid.

Horizontal Grid Refinement

Horizontal child grid refinement involves specifying the location of the child grid within the parent grid, and defining the row and column refinement ratio.

Define Numerical Grid	Contraction in state of	the setting of the				
Name: Child grid1						
Define Horizontal Grid Refinement Ratio: 3:1 Row Refinement Start: 1 End: 1	Preview Column Refinement Start: 1 End: 1 Add Data Object					
				Back</td <td>Next >></td> <td>Cancel</td>	Next >>	Cancel
Tip!	You can add data maps) from the da to assist you in de grid within the par objects from the c	ata explore etermining f ent grid. S	r to the 2D he placem elect the d	Viewer p nent of the lesired da	preview e child ta	

Enter a unique name for the child grid in the Name field.

Next, select the refinement ratio from the Ratio combo box. A ratio of 3:1, for example, will refine the parent cell by a factor of three, resulting in nine horizontal child cells within one parent cell.

displayed in the 2D Viewer preview.

Finally, specify the Row Refinement interval and the Column Refinement interval, by selecting the starting row/column and ending row/column, for where the grid refinement should be applied within the parent grid. The child grid can be placed anywhere within the parent grid as long as it does not overlap another child grid.

Please Note: The child grid cannot be rotated; it must be in the same orientation as the parent grid.

Click the [Preview] button to preview the child grid in the adjacent 2D Viewer.

Click the [Next] button to proceed to the next step.

Vertical Grid Refinement

Vertical grid refinement involves selecting which model layers to refine and specifying the refinement ratio for the selected layers.

🐯 Define Numerical Grid	Construction in the local division in the lo	providence (
Define Vertical Grid Refinement Specify End Layer				
Start				
End 2				
Refinement ratio				
Globally for all layers 1:1	•			
Specify for each layer				
1 2	1:1			
			< <back finish<="" td=""><td>Cancel</td></back>	Cancel

The top of the child grid must always coincide with the parent grid and therefore the Start layer will always be 1. However, the End layer can be any model layer below the top model layer in the simulation domain.

There are two options for defining the refinement ratio. Select Globally for all layers to assign a single refinement ratio to all layers. Alternatively, select Specify each layer to assign a refinement ratio layer by layer.

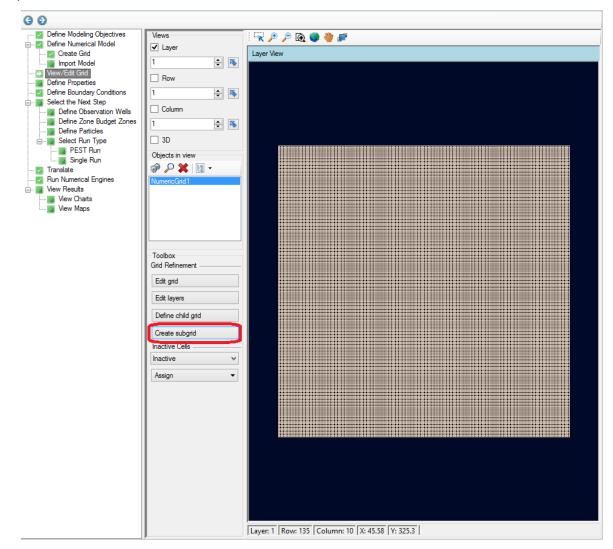
Please Note: Although the top layer must be the start layer, vertical refinement does not have to start at the top. Assign a refinement ratio of 1:1 to the top layer and it will not be refined.

Click the [Finish] button to create the child grid.

8.1.4 Extract Subgrid

When working with large regional models, you may find it difficult to manage as model runtime(s) can be quite long and associated files can become quite large. Additionally, you may be interested in doing further modeling - but only for a smaller area of the large regional model. Extracting a subgrid from your regional model allows you to work with a smaller model focused on an area of interest.

You will find the option to **create a subgrid** in the Numerical Workflow on the View/Edit Grid step.



Additionally you have the option to extract a subgrid from an existing grid (which has been run) by right clicking on the existing grid in the Model Explorer and selecting Extract subgrid...

By extracting a subgrid - all existing inputs (for example: inactive cells, properties, boundary conditions, observation wells, zone budget zones, and particles) that are in the existing grid will be transferred to the subgrid. Outputs are not transferred.

Extracting Subgrids
Visual MODFLOW Flex only supports extracting subgrids from Finite Difference grids. USG and Finite Element grids do not support extracted subgrids.
The model on the grid you are trying to extract a subgrid from must have been translated and run to completion and only the following engines are supported:
 MODFLOW 2000 MODFLOW 2005 MODFLOW-NWT MODFLOW-6

The following dialog appears when selecting Create subgrid...

	Extract subgrid	-		×
Subgrid details Script				
Subgrid name	Layer 1 📑 🐺 🥕 🔎 🍖 👋			
NumericalGrid1_subgrid				
Row				
Start:				
25				
End:				
<mark>75</mark>				
Column				
Start:				
25				
End:				
75				
Layer				
Coming soon in a future release				
Start:				
1 📫			##	
End:				
2			▦	
Highlight dry cells	Row: 64 Column: 3 X: 1682.35 Y: 7805.88 Cell width: 130 Cell h	eight: 1	30	
	Add objects using the Data and Model Explorer tree checkboxes			
	<u>O</u> K <u>C</u> ancel		Help	

By default a Subgrid name will be provided but you can adjust this.

You can adjust the Row start and end as well as the Column start and end to define your subgrid.

It may be helpful to load objects (from the Data and Model Explorer) to help you define your subgrid - simply select the appropriate checkbox and they will be displayed in the subgrid preview in this dialog - for example a River has been added to the subgrid preview in the above image.

Currently all Layers will be included in your subgrid. In future versions you will be able to a select a subset of layers to include in your subgrid.

You can highlight the dry cells in your model display in the subgrid preview. This can be helpful to ensure that no dry cells land on the boundary of your subgrid.

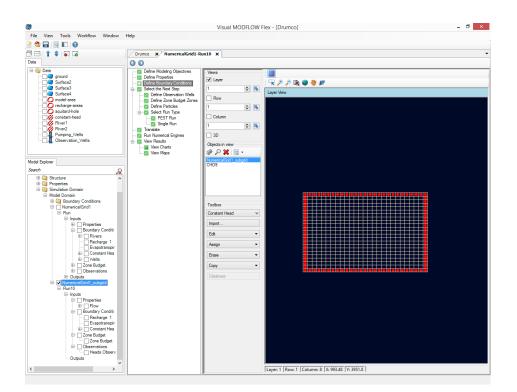


Please be aware that the boundary of your subgrid cannot fall on cells that are dry (from the regional model run). You must adjust the extents of your subgrid to ensure no dry cells fall on the boundary.

The toolbar at the top of the subgrid preview provide+s you with several options:

- 🔹 🥕 Zoom In
- 🎤 Zoom Out
- 🖻 Zoom to Box
- Zoom to Full Extent
- 🖑 Pan

Once you have defined your subgrid extents and select OK you will find the new subgrid (with corresponding model) will appear in the Model Explorer as well as a new Numerical Workflow will open. Select the subgrid in the Model Explorer to have it display in the new Numerical Workflow.



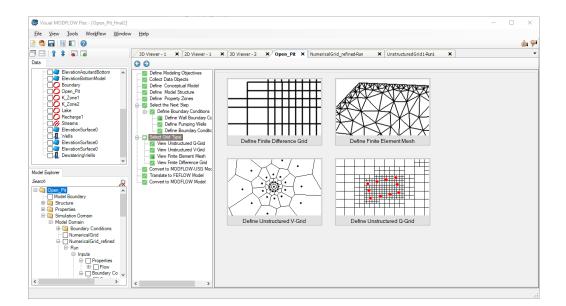
As mentioned previously, all inputs from the original grid will be transferred to your subgrid. Additionally, the subgrid will contain constant heads all the way around the perimeter with assigned heads values from the original model. From here you can continue to develop your new model based on your subgrid extraction.

8.2 Define Finite Element Mesh

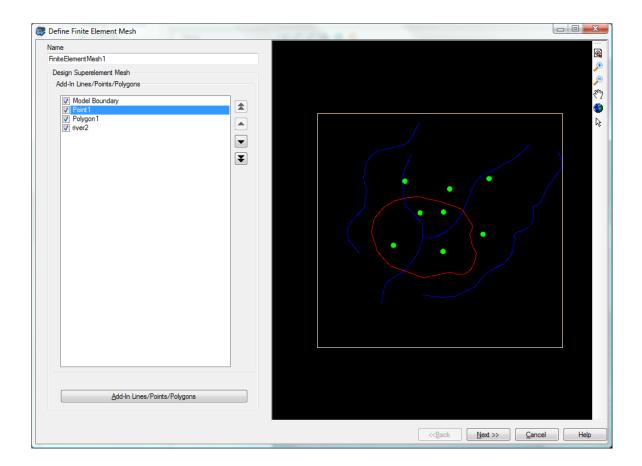
Quick Overview

Instructions	Create the superelement mesh, define the mesh size, and define vertical layering type and resolution
Pre-requisites:	The Conceptual Model has been defined.
Result:	A finite element mesh is created
Next Steps:	Convert Conceptual Model to FEFLOW finite element model

From the "Select Grid Type" step in the Conceptual Model workflow, click on the "Define Finite Element Mesh button":



The Define Finite Element Mesh wizard will appear on your screen, where you can configure the properties of the finite element mesh.

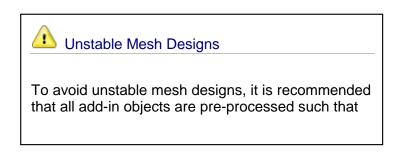


Specify a unique name for the finite element mesh in the Name text field.

Defining the Superelement Mesh

The Superelement Mesh represents the main geometry (points and segments) of the model region from which finite elements are generated. A superelement mesh is defined using the model boundary polygon geometry and, optionally, one or more "add-ins". Add-ins are lines, points or polygons within the model boundary which Visual MODFLOW Flex uses as focal points to create nodes during finite element mesh creation.

By default, the Add-ins List contains the model boundary and any linear or point boundary condition currently defined for the conceptual model. Additional add-ins may be added to the list using data objects from the Data Explorer.



the following conditions are met:

- there is relatively equal spacing between vertices along polylines and the edges of polygons,
- polygons in the same layer do not overlap or contain slivers, and
- vertices in all added layers that appear to share common coordinates share them exactly

Data object geometry can be edited using the 2D Viewer editing tools. For more information, please see "Digitizing & Editing Geometry in 2D Viewers".

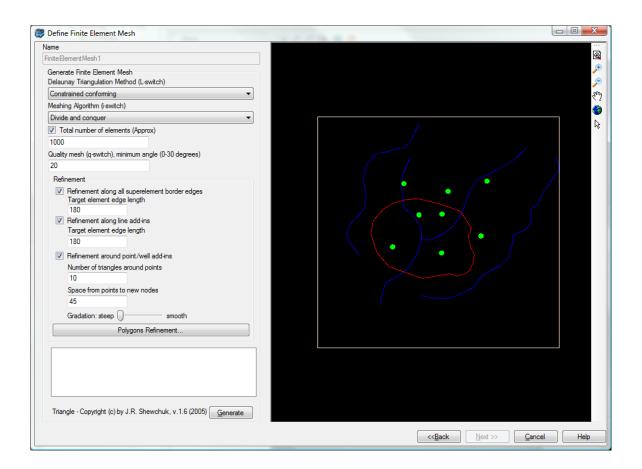
To add an Add-In features using a data object from the Data Explorer,

- Leaving the Define Finite Element Mesh window open, select the desired data object from the Data Explorer.
- In the Define Finite Element Mesh window, select the Add-in Lines/Points/Polygons button, located below the Add-ins List .

An Add-in may be included or excluded in the mesh creation, by checking or unchecking the corresponding check box, respectively. When an add-in is "checked" it will also be displayed in the adjacent 2D Viewer preview window.

Defining the Horizontal Mesh Settings

In the second dialog in the Define Finite Element Mesh wizard, you can define various discretization settings for the horizontal mesh.



Finite element meshes are created using the Triangle mesh generator, developed by J.R. Shewchuk (<u>1970</u>). Triangle provides various options for generating finite element meshes. These options are described briefly below.

Please Note: the switch letters in parenthesis beside the name of each option refers to the command line switches used by the Triangle mesh generator.

Delaunay Triangulation Method (L-switch)

Delaunay triangulation methods are typically used in finite element mesh generation as they tend to maximize the minimum angle of all the angles of the triangles in the triangulation, providing a nice set of triangles, and avoiding narrow "skinny" triangles. There are three triangulation methods from which to choose from: Constrained, Constrained Conforming and Conforming.

- **Constrained**: Triangulation in which each segment appears as a single edge in the triangulation. As such, segments are not subdivided, and new vertices are not added to the vertex set. A constrained Delaunay triangulation is not truly a Delaunay triangulation, because some of its triangles might not be Delaunay.
- **Constrained Conforming**: Triangulation in which triangles are constrained Delaunay; however, additional vertices may be added to the vertex set and segments may be subdivided to ensure a user-defined Minimum Angle constraint is satisfied. If a minimum angle is not specified, vertices are added to ensure all angles are between 20 and 140 degrees.

• **Conforming**: Triangulation in which each triangle is truly Delaunay, and not just constrained Delaunay. Additional vertices may be added to the vertex set to enforce the Delaunay property.

Meshing Algorithm (I-switch)

Two Delaunay algorithms are provided for generating the finite element mesh: Divide and Conquer, and Incremental. Typically, the divide and conquer algorithm is preferred. However, if this algorithm fails, use the incremental algorithm.

Total Number of Elements (Approx)

For the Conforming and Constrained Conforming triangulation methods, you can specify the desired number of elements that comprise the finite element mesh. Please note that the specified number of elements cannot be less than the default number generated by Triangle, i.e., the number generated if this option is disabled.

Minimum Angle

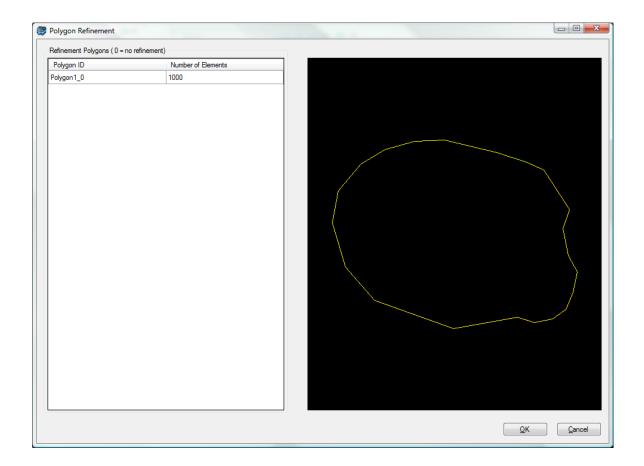
For the Constrained Conforming triangulation method, a minimum angle can be specified. The specified angle will replace the default bound on the minimum angle (20 degrees). The specified angle may include a decimal point, but cannot be expressed in exponential notation.

Refinement Options

- Edges of triangles along model boundary should have approx length: Use this option to set the approximate length of edges (segments) that comprise the model boundary domain. Vertices will be added along the boundary, creating subsegments with the specified length. This option will refine the areas along the model domain boundary.
- Edges of triangles along line should have approx length: Use this option to set the approximate length of edges of triangles along line add-ins. Vertices will be added along the lines, creating subsegments with a specified length. The option will refine areas around line add-ins.
- **Refinement around point add-ins**: Use this option to refine areas around point addins. Refinement for point add-ins is defined by specifying the number of triangles directly around the points, and the desired distance from the point to the new vertices. Use the Gradation slider bar to specify the smoothness of the transition from the fine elements around the points to the coarser elements. A smoother transition will result in more elements, but will lead to more regular elements therefore improved model stability.

Polygon Refinement

You can use one or more polygon data objects that have been included in the superelement mesh (see "<u>Create Finite Element Mesh</u>) to define localized areas of mesh refinement. To do so, click the Polygons Refinement... button. The Polygon Refinement screen will appear.



In the left side of the Polygon Refinement window, all features in the polygon add-ins are listed in a table under the Polygon ID column. When a feature is selected, it is highlighted yellow in the adjacent 2D Viewer. Select the polygon feature that represents that area of the mesh for which refinement is to be performed. In the adjacent field under the Number of Elements column, enter the desired number of element that should exist in polygon area. Visual MODFLOW Flex will automatically refine the underlying triangles to equal the prescribed number of elements for the polygon area.

Once you have defined the refinement for the polygon features, click the [OK] button to apply the settings.

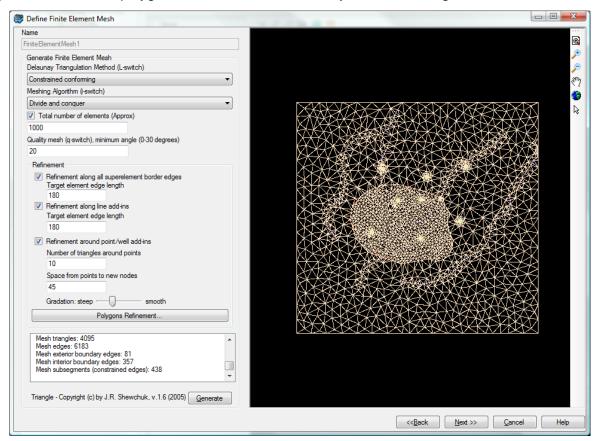
Generating the Horizontal Mesh

Once the above settings have been defined, click the [Generate] button to generate the horizontal mesh. Once generated, the Triangle output results, e.g., number of mesh vertices, triangles, edges, etc, are displayed in the text box (above the Generate button). These results may be copied to the clipboard by right-clicking anywhere inside the box, and selecting Copy to Clipboard from the pop-up menu.

The generated mesh will also display in the adjacent 2D Viewer window.

If you are not satisfied with the mesh, you can modify the settings and regenerate the mesh by selecting the Generate button again.

If you have selected polygon refinement, the mesh may look something similar to below.



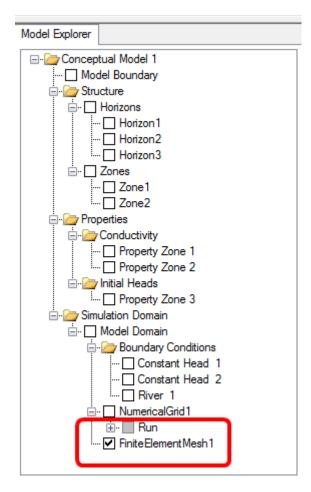
Defining Slice Elevations

The third step in the finite element mesh creation involves defining slice elevations. Various settings are available for defining the slice elevations in the third dialog of the finite element mesh creation wizard (shown below).

efine Slice Elevations		
Mesh Type		
Deformed	•	
Number of Layers	Zmin	
10	41.527	
Min Layer Thickness	Zmax	
0.1	365.988	
Description In a deformed grid/mesh, the	tops and bottoms of the model layers s. You can refine the model layers, by tionately thick layers.	
Layer Name	Layer Refinement	
Zone1	1	
	1	
Zone2		
	1	
Zone3	1	
Zone3 Zone4	1 1 1	δ
Zone3 Zone4 Zone5	1	
Zone3 Zone4 Zone5	1	Real Provide American Street Provide Amer
Zone3 Zone4 Zone5	1	
Zone2 Zone3 Zone4 Zone5 Zone6	1	
Zone3 Zone4 Zone5	1	
Zone3 Zone4 Zone5	1 1 1	
Zone3 Zone4 Zone5	1	Exaggerate 33

The options available for defining slice elevations are similar to those for defining slice elevations for finite difference grids. For information on these settings, e.g., grid types, min layer thickness and layer refinement, please refer to "<u>Defining the Vertical Grid</u>".

Once the vertical mesh settings have been defined, click the [Finish] button to generate the finite element mesh. The finite element mesh will now appear in the Model Explorer tree under the Model Domain node as shown below, where it can be displayed in a 2D or 3D Viewer window, and used in <u>Translation to Finite Element Model</u>.



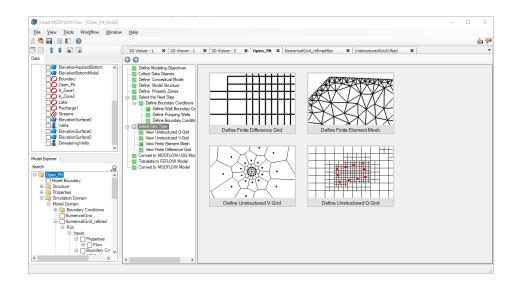
Define Unstructured Voronoi Grid 8.3

Quick Overview

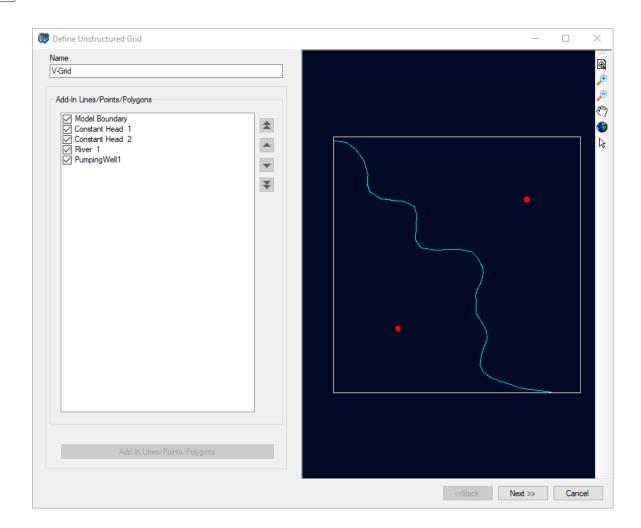
Instructions	Define add-ins for the grid, define the approximate number of cells, and the refinement options.
Pre-requisites:	The Conceptual Model has been defined.
Result:	An unstructured Voronoi Grid is created and added to the Model Explorer tree.
Next Steps:	Convert Conceptual Model to MODFLOW-USG

For more details on how MODFLOW-USG differs from traditional versions of MODFLOW, please see our website.

From the "Select Grid Type" step in the Conceptual Model workflow, click on the "Define Unstructured V-Grid" button:



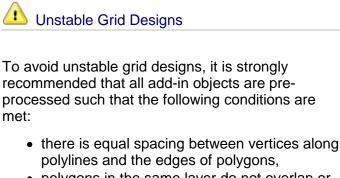
The Define Unstructured V-Grid wizard will appear on your screen, where you can configure the inputs for the grid.



Specify a unique name for the unstructured V-Grid in the Name text field.

Defining the Grid Add-Ins

The Add-ins for the grid represents the main geometry (points and line segments) of the model region from which Voronoi Cells are generated. The add-ins consist of the model boundary (a closed polygon) and, optionally, one or more "add-ins". Add-ins are polylines, points, or polygons within the model boundary which Visual MODFLOW Flex uses as "node generators" for the grid generator. By default, the Add-ins List contains the model boundary and any linear or point boundary conditions defined for the conceptual model. Additional add-ins may be added to the list using data objects from the Data Explorer. Boundary conditions that are created with polygons are not included in the Add-Ins, by default. (Generally, it is not recommended to include polygon-based boundary conditions that cover the entire model, as grid add-ins; (for example, recharge or evapotranspiration. However, smaller polygons, for example those representing lakes, ponds, drains, general heads, etc., may be used)



- polygons in the same layer do not overlap or contain slivers, and
- vertices that appear to share common coordinates share them *exactly*

Data object geometry can be edited using the 2D Viewer editing tools. For more information, please see "Digitizing & Editing Geometry in 2D Viewers".

To add an Add-In feature using a data object from the Data Explorer:

- Select the desired data object from the Data Explorer (while leaving the Define Unstructured Grid window open)
- In the Define unstructured grid window, select the [Add-in Lines/Points/Polygons] button, located below the Add-ins List .

An Add-in may be included or excluded in the grid creation, by checking or unchecking the corresponding check box, respectively. When an add-in is "checked" it will also be displayed in the adjacent 2D Viewer preview window.

When you are finished, click the [Next>>] button to proceed.

Defining the Grid Size and Refinement Settings

In the second dialog, you can define various settings that control the cell sizes and the approximate number of cells.

ame		 	
-Grid			
Define Unstructured Grid Delaunay Triangulation Method (L-switch)			
Force all triangles to be Delaunay			
Meshing Algorithm (i-switch)			
Divide and conquer			
Total number of elements (Approx)	$\langle \rangle$		
Quality mesh (q-switch), minimum angle (0-30 degrees) 30		•	
Refinement			
 Refinement along all superelement border edges Target element edge length 192 Refinement along line add-ins Target element edge length			
Gradation: steep			
Layer Refinement Settings			
Triangle - Copyright (c) by J.R. Shewchuk, v.1.6 (2005)			

Unstructured grids are created using the Triangle mesh generator, developed by J.R. Shewchuk (<u>1970</u>). Triangle provides various options for generating unstructured grids. These options are described briefly below. Please note that the switch letters in parenthesis beside the name of each option refers to the command line switches used by the Triangle mesh generator. More details on "Triangle" are available on the <u>Triangle website</u>.

In Visual MODFLOW Flex, this mesh generator is used to create a Delaunay Triangulation, and from this, Voronoi Grid cells are created, which are suitable grids for MODFLOW-USG. More details on Voronoi Polygons and grids can be found <u>on our website</u>.

Delaunay Triangulation Method (L-switch)

Currently this option is always set to Force all triangles to be Delaunay.

Meshing Algorithm (I-switch)

Two Delaunay algorithms are provided: *Divide and Conquer*, and *Incremental*. Typically, the divide and conquer algorithm is preferred. However, if this algorithm fails, use the incremental algorithm.

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Total Number of Elements (Approx)

This setting is a target for the grid generator, and is an approximation of how many cells will comprise the areas outside the refinement regions. The actual total number of cells generated in the grid will depend on the geometry add-ins you have included, and the refinement settings, and will typically be much higher. For example:

- In the figure above there are 2 wells, and 3 polyline boundaries. Using the default refinement settings and the number of elements as 1000 results in approximately 4300 unstructured grid cells (per layer).
- For the same example, using 10000 as the total number of elements, 100 for the edge length around lines, and 25 as the spacing from points to new nodes, and middle-range Gradation, results in 19000 unstructured grid cells (per layer).

As a rule-of-thumb, the actual number of Voronoi cells that will result from the grid generator is typically within the same order of magnitude as the value you define for the "Total Number of Elements".

Fortunately in Visual MODFLOW Flex, you can repeat the grid generator several times, create multiple grids, and find the most suitable grid size and refinement level for your project.

Quality Mesh (Minimum Angle)

The default is 30 degrees for creating Voronoi polygons, and should be suitable in most cases. However, if you encounter difficulties with the default value, you may experiment with values of 15 or 20 degrees. In theory, values with lower angles may work, though we have limited testing experience with these geometries.

Refinement Options

The refinement options are separated into three categories, each of which can have its own unique refinement levels:

- Superelement border edges: (the conceptual model boundary)
- Line add-ins (linear boundary conditions such as constant heads, rivers, drains, etc.)
- Point (well) add-ins

For each of the refinement settings, you enter an "edge length" (defined using the same unit convention as the project's units), and this will result in an "equivalent" approximate cell size.

• **Refinement around superelement border edges**: Use this option to set the approximate length of edges (segments) that comprise the model boundary domain. Vertices will be added along the boundary, creating subsegments with the specified length. This option will refine the areas along the model domain boundary.

- **Refinement around line add-ins**: Use this to set the approximate target cell size around the polyline add-ins. Vertices will be added along the lines, creating subsegments with a specified length. The option will refine areas around line add-ins.
- Refinement around point/well add-ins: Use this option to refine the grid around point add-ins. Refinement for point add-ins is defined by specifying the number of triangles directly around the points, and the desired distance from the point to the new vertices. The default of 10 triangles should be adequate for most cases; in order to adjust the cell size around the pumping wells, you need to change the "Space from points to new nodes" value; a smaller value will result in smaller cell sizes.
- Gradation: Use the Gradation slider bar to specify the smoothness of the transition of the cell sizes from around the refinement regions to the more coarser (background) cell sizes. A smoother transition will result in more cells, but will lead to a more gradual change in cell size, which is recommended for MODFLOW-USG grids.

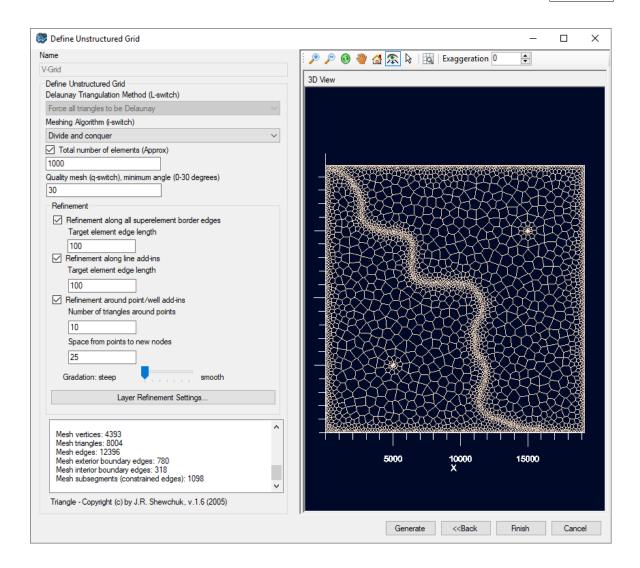
Layer Refinement

You can refine the conceptual layers of the model into sub-layers using the Layer Refinement Settings button, which opens a window with a table and allows you to specify the number of evenly divided sub-layers for each conceptual layer in your model.

Unstructured Grid Layer Refinement		_		\times
Define Slice Elevations Description For unstructured grids, layer refinement de During deformed grid/mesh refinement, in and bottoms of the newly created layers for	put layers are proportion	ately refined	, while top	s
Layer Name Zone 1	Layer Refinement			
Zone2	2			
1	opply Settings	Ж	Cance	ł .:

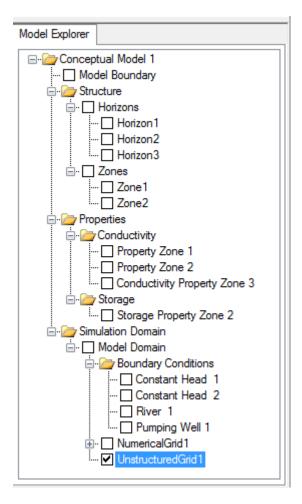
Generating the Grid

Once the above settings have been defined, click the [Generate] button to generate the unstructured grid. Once generated, the Triangle output results, e.g., number of mesh vertices, triangles, edges, etc, are displayed in the text box (above the Generate button). These results may be copied to the clipboard by right-clicking anywhere inside the box, and selecting Copy to Clipboard from the pop-up menu.



The generated grid will also display in the adjacent 3D Viewer window. If you are not satisfied with the grid, you can modify the settings and regenerate the grid by selecting the [Generate] button again.

Once the grid is defined, click the [Finish] button to complete the process. The unstructured V-Grid will now appear in the Model Explorer tree under the Model Domain node as shown below, where it can be displayed in a 3D Viewer window.



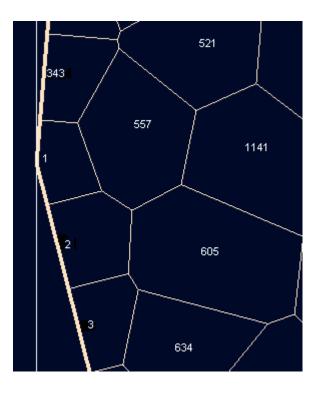
Next you are ready to generate a numerical model from this unstructured Grid. This is explained in the section <u>Converting to MODFLOW-USG</u>.

When you are done previewing the grid, click on the 🐑 Next button on the workflow toolbar.

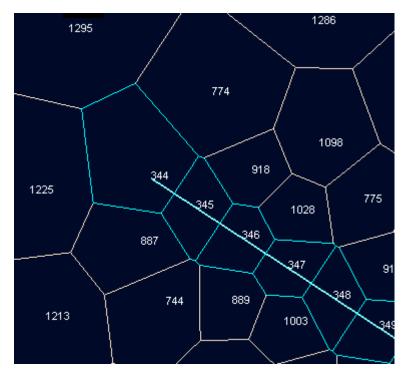
8.3.1 Cell Numbering

The order in which cells are numbered for unstructured Voronoi grids is as follows.

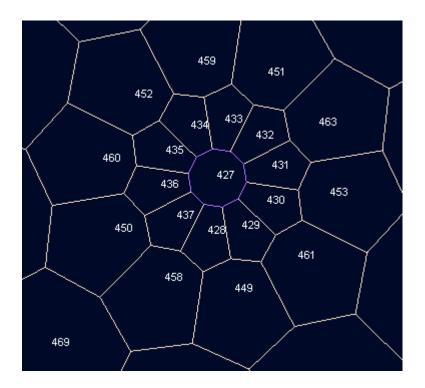
1.CellID 1 starts at the first vertex of the model boundary polygon in the uppermost layer and works along the edge (typically in a counter-clockwise direction



2. After this, the add-ins are numbered, starting with polylines, then polygons. Vertices of the shapes are numbered based on their order:



3. Then point features (including wells) and the specified number of neighbors are added:



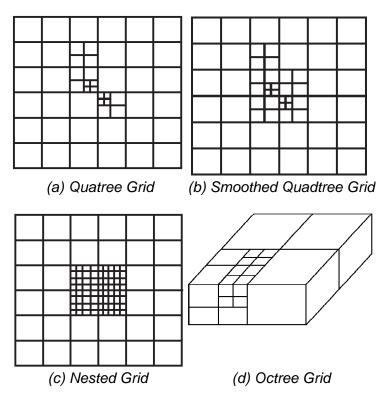
4. After this, the remaining cells are numbered, filling in the gaps, starting with layer 1, and working downwards.

8.4 Define Unstructured QuadTree Grid

Quick Overview

Instructions	Define add-ins for the grid, define the approximate number of cells, and the refinement options.
Pre-requisites:	The Conceptual Model has been defined.
Result:	An unstructured Q-Grid is created and added to the Model Explorer tree.
Next Steps:	Convert Conceptual Model to MODFLOW-USG

Quadtree grids are based on rectangular-shaped grid cells that can be sequentially subdivided into four equally-sized cells. Quad-Based grid refinement is a simple way to focus resolution in areas of interest in order to better represent hydraulic gradients or to more accurately represent known variations in hydraulic properties or boundary conditions.

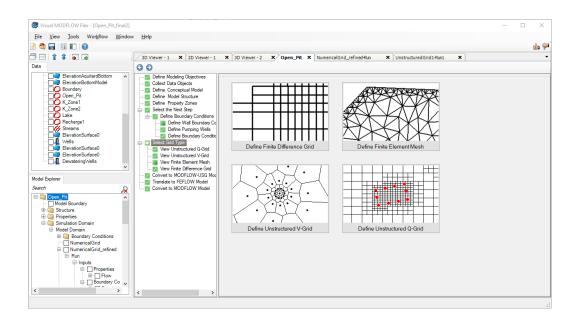


Examples of Quad-Based grids include Nested grids, Quadtree grids, and Octree grids (the case when a Quadtree grid is variably-refined in three dimensions).

Images adapted from Panday (2013)

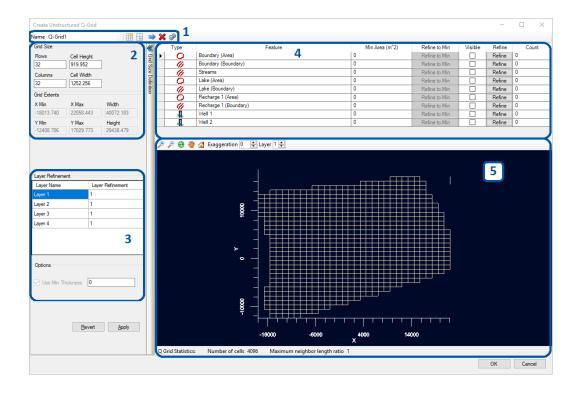
In order to reduce numerical errors and improve accuracy of the simulation, it is generally recommended that Quad-Based grids are smoothed so that every cell is connected to no more than two cells in any direction. Doing so can simplify the calculation of the Ghost Node locations (for the Ghost Node Correction [GNC] package). Also, keeping with a limit of two connections per cell face may yield minimal errors in the calculated heads/fluxes such that the GNC package may not be needed. For more details on how MODFLOW-USG differs from traditional versions of MODFLOW, please see our <u>website</u>.

From the "Select Grid Type" step in the Conceptual Model workflow, click on the "Define Unstructured Q-Grid" button:



The Define Unstructured Q-Grid wizard will appear on your screen, where you can configure the inputs for the grid. There are five groups of controls in the wizard:

- 1. Toolbar
- 2. Grid Size
- 3. Layer Refinement
- 4. Feature Refinement
- 5. Viewer and Statistics



Toolbar

The toolbar includes the following controls:



Name: Specify a unique name for the Unstructured Q-Grid.

Reset Refine: resets the grid to the Grid Size settings and removes all feature refinement and smooth operations

Smooth: refines cells that have four or more neighbors along the same cell face

Add Selected Feature: adds a feature selected in the Data Explorer to the refine Feature Refinement control

Delete Selected Feature: deletes the selected feature from the Feature Refinement control

Settings: provides visualization settings for the selected feature in the Viewer

Defining the Grid Size

By default, Visual MODFLOW Flex discretizes the Q-grid layers into 32 rows and 32 columns. The Columns and Rows fields allow you to define the base grid size. You can also specify the Cell Height and Cell Width; the Rows and Columns (and potentially the extents) will be updated accordingly.

Grid Size				
Rows	Cell Height 453.927			
Columns	Cell Width			
32	478.482			
Grid Extents				
X Min	X Max	Width		
481897.382	497208.800	15311.418		
Y Min 4867005.309	Y Max 4881530.982	Height 14525.673		

Defining the Vertical Grid

The Layer Refinement controls allow you to subdivide the conceptual layers into the specified sublayers. All layers will be deformed.

Layer Refinement	
Layer Name	Layer Refinement
Layer 1	1
Layer 2	1
Layer 3	1
Layer 4	1
Layer 5	1
Layer 6	1
Options Use Min Thickness	

The optional use minimum thickness option allows you to specify a threshold thickness below which cells will be removed from the model. This can help remove isolated or socalled island cells from thin layers that may cause numerical instabilities.

Cells within pinchout areas of structural zones and cells below the specified minimum thickness will be inactivated such that vertical connections are passed through these cells.

Defining the Grid Size and Refinement Settings

Features can be refined at locations where the grid intersects selected polygons \mathcal{O} , polylines \mathcal{M} , points \mathfrak{P} or well \P objects from the Conceptual Model Boundary Conditions and Data Explorer objects.

	Туре	Feature	Min Area (m^2)	Refine to Min	Visible	Refine	Count
Þ	0	Boundary (Area)	0	Refine to Min		Refine	0
	4	Boundary (Boundary)	0	Refine to Min		Refine	0
	4	Streams	0	Refine to Min		Refine	0
	0	Lake (Area)	0	Refine to Min		Refine	0
	4	Lake (Boundary)	0	Refine to Min		Refine	0
	0	Recharge 1 (Area)	0	Refine to Min		Refine	0
	4	Recharge 1 (Boundary)	0	Refine to Min		Refine	0
	4	Well 1	0	Refine to Min		Refine	0
	4	Well 2	0	Refine to Min		Refine	0
	23	ElevationSurface	1	Refine to Min		Refine	0

By default, all of the boundary conditions assigned in the conceptual model are included in the Refine Features table. Polygons that are added to the table, also have their (polyline) boundaries added so that you can refine the edge of the polygon and/or its interior. Additional features can be added from the Data Explorer to the table using the Add Selected Feature solution.

To refine the grid around a selected feature, click the Refine button. You can click the Refine button several times to refine the grid sequentially. You can also set a threshold value for the Min Area field of a given feature (in project length-squared units). When a non-zero value is set, you can sequentially refine the model until refining operation(s) would lead to grid cells smaller than this threshold area. Once a non-zero value has been specified, you can also automatically refine the grid near the selected feature by clicking the

Refine to Min	button which iterati	vely refine	es all inter	secting cells u	ntil a subdivisio	n
	d cause a grid cell a					
Area value app	lies to both the the	Refine	and the	Refine to Min	buttons.	

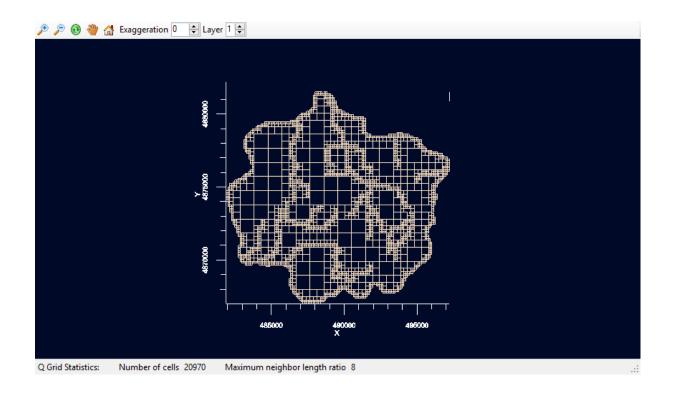
Please Note: The automated grid refinement using the Refine to Min button can be fairly slow for operations involving large grids, features with many vertices, and/or low specified Min Area values and may require some time to complete as each refinement step will quadruple the number of cells that intersect the selected feature(s). You can stop the automated refinement process part-way through the operation and it will complete the current iteration by clicking the stop button.

The Refine Features table also contains a Visible field which toggles the visibility of the features in the Preview window below the table and a Count field which indicates how many times the feature has been refined.

Q-Grid Preview

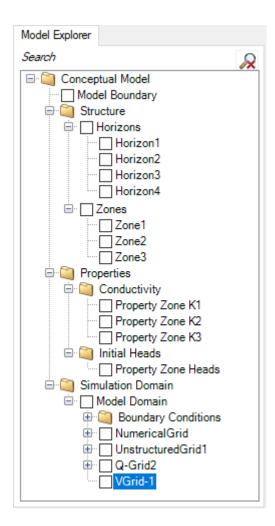
A preview of the Q-Grid will be displayed in the 3D Viewer window in the lower right quadrant of the Defined Q-Grid window. If you are not satisfied with the grid, you can modify the settings and regenerate the grid by selecting the Reset Refine button. A status bar can be found at the bottom of the preview window that indicates the total number of grid cells based on the current settings as well as the Maximum neighbor length ratio. This ratio

indicates the largest relative difference in length or width between adjacent connected cells. As discussed above, a lower ratio may reduce errors in solving the flow equation and a value of 2 is generally ideal. You can refine cells that are four or more times wider/longer than a neighbor by clicking the smooth button. If the adjacency ratio is larger than 4, you may need to smooth the grid several times.



Finishing the Design

Once the grid is defined, click the [Finish] button to complete the process. The unstructured Q-Grid will now appear in the Model Explorer tree under the Model Domain node as shown below, where it can be displayed in a 3D Viewer window.



Next you are ready to generate a numerical model from this Unstructured Q-Grid. This is explained in the section <u>Converting to MODFLOW-USG</u>.

When you are done previewing the grid, click on the Solution on the workflow toolbar.

9 Converting Conceptual Models to Numerical Models

Visual MODFLOW Flex allows you to translate your conceptual model to one or more numerical models that will run in a groundwater modeling engine. Finite difference and finite control volume models can be run and analyzed within the Visual MODFLOW Flex environment, while finite element models are exported to run in <u>FEFLOW</u>. During translation, Visual MODFLOW Flex automatically populates the specified grid or mesh with the defined geological formations, boundary conditions, and property zone attributes, and creates the necessary input files for loading into your desired simulator.

Separate workflows will be generated every time a conceptual model is converted into a numerical model. Structured finite difference grids (which work with the following engines: MODFLOW-2000, -2005, -NWT, -LGR, - SURFACT, SEAWAT, MT3DMS, and RT3D) are converted to the <u>numerical workflow</u>, while unstructured finite control volume grids are converted to the unstructured grid <u>USG workflow</u>. In each workflow, you can view/edit the properties and boundaries on the numerical grid, then translate and run a groundwater modeling engine and view the results.

For finite element models, Visual MODFLOW Flex will generate the .FEM problem file for loading into FEFLOW.

Please Note: FEFLOW v.5.4 or later is required for opening and running FEFLOW models.

This chapter walks you through the steps involved in translating a conceptual model to a numerical model, and includes information on the following topics:

- <u>Converting to MODFLOW-Finite Difference</u>
- <u>Converting to MODFLOW-USG</u>
- Converting to FEFLOW

9.1 Converting to Structured Grid Numerical Model (MODFLOW-2000/2005/6)

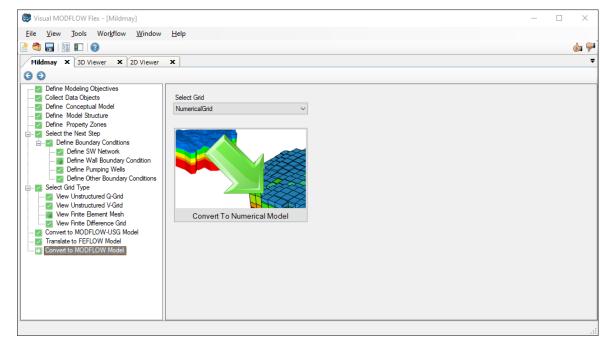
Quick Overview

Instructions	Create a MODFLOW numerical model by populating the selected grid with data from the conceptual model
Pre-requisites:	A Finite Difference Grid has been created.
Result:	A numerical model is generated and added to the Model Explorer tree. The numerical model workflow will appear.

Next Steps: Numerical Modeling Workflow

Once you have the conceptual model designed and at least one numerical grid, you are ready to populate this grid with the conceptual data.

Proceed to the "Convert to Numerical Model" step in the Conceptual Model workflow as shown below.



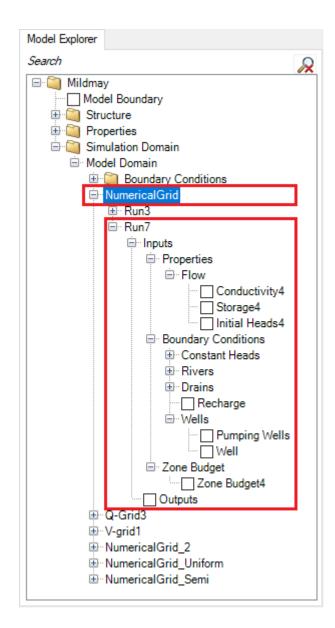
The Select Grid combo box will list all the finite difference grids you have created for your project, including grids for use in Local Grid Refinement (LGR).

Select the grid you wish to use ,and click on the "Convert to Numerical Model" button. (Alternatively, you can select the desired numerical grid from the Model Explorer tree, right mouse click, and select "Convert to Numerical Model from the pop-up menu.)

After clicking on the conversion button, a new numerical model workflow window will appear which includes the steps for the numerical model. In the first window, you will see the progress of the conceptual to numerical conversion. This conversion could take several minutes, depending on the size and type of grid you used, and the complexity of the conceptual model inputs.

Mildmay X 3D Viewer X 2D	Viewer × NumericalGrid-Run7 Numerical Hodel ×					
00						
Define Modeling Objectives	Row type	Transport Active				
- Define Boundary Conditions	Saturated (Constant Density)	Retardation Model				
Select the Next Step Define Observations	Simulation type	No sorption simulated				
- Define Zone Budget Zones	Groundwater Row V	Reaction				
Define Particles Select Run Type		No kinetic reactions				
PEST Run	Available Row Engines USSS MODFLOW 2005 from WH USSS MODFLOW 2005 from WH	Available Transport Engines				
- Single Run Translate	MODELOW-6	MICONS MODELOW-SURFACT				
Run Numerical Engines	USGS MODFLOW - LGR from WH MODFLOW-NWT	MODFLOW-SURFACT MODFLOW-6				
Wew Results Wew Chats	NODFLOW-SURFACT from HGL NODPATH					
View Maps	mod-PATH3DU from SSPA Zone Budget					
	Long bodger					
	Start Date	Species Parameters Model Parameter	9			
	Fiday , January 1, 2010	+ X				
	The Start Date corresponds to time = 0 in your numerical model. This value cannot be changed once it has been set.	Name	Description	Mobile	InitialConcentration (mg/L)	MDCOEF (m "2/day)
		Conct01	Concl01	2	0	
	Default Project Property Settings					
	21 21					
	Conductivity Nx (m/s) 0.0001		Conversion Progress			
	Ky (m/s) 0.0001		concatorrogica			
	Kz (m/s) 1E-05		Converting Properties:			
	Initial Heads (m) 100 V Storage		Converting property for conductivity Cond-L1 Converting property for conductivity Cond-L2 Converting property for conductivity Cond-L3 Converting property for conductivity Cond-L4			
	Effective Porosity 0.14		Conveting property for conductivity Cond-L4 Conveting property for conductivity Cond-L5			
	Sa (1/m) 1E-05 Sy 0.2		Converting property for conductivity Cond-L5 Converting property for initial_heads Initial Heads			
	Total Porosity 0.3		Conductivity			
			Storage Initial Heads			
			Specified Head			
			River 1			
			Recharge Record Walls			
			Well Conceptual model to numerical model conversion	has considered *****		
			1			
				Close		
				_		
	Effective Porosity	1				
	Effective Porosity					
		Name (Caption)				

During the conversion, the run node will be added to the model explorer under the numerical grid that you selected. This tree will be populated with all the inputs from your conceptual model: Properties, Boundary Conditions, Wells, etc. A grid may have multiple run nodes to facilitate simulating multiple scenarios in the PRO and Premium versions of Visual MODFLOW Flex. For more information on working with multiple model scenarios in a project, please see the section on Working with Multiple Model Scenarios.



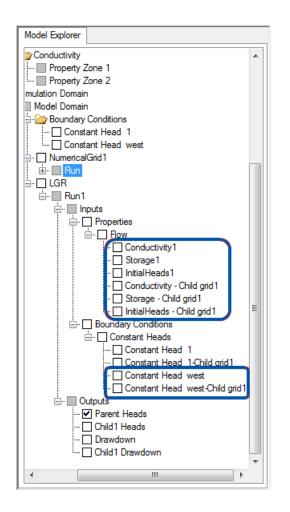
When the conversion is complete, you can click on the S Next button on the workflow toolbar, which will take you to the <u>Define Properties</u>. You can then proceed through the <u>numerical model workflow</u>.

Converting MODFLOW Grids with Child Grids

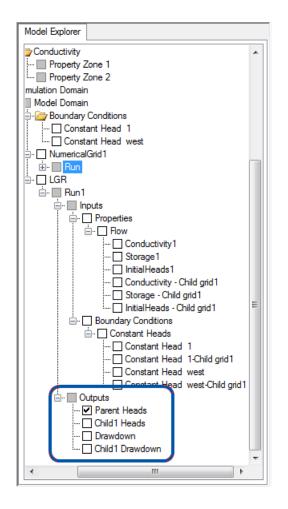
When you convert a Grid that contains one or more child grids (for an LGR run), the inputs on the Model Explorer tree will contain objects for the parent model and each child model.

In the example below, Conductivity1, Storage1, InitialHeads1 are the property values for the *Parent* Grid and Conductivity-Child grid1, Storage - Child grid1, and InitialHeads - Child grid 1 are the property values for ChildGrid1.

The same convention applies for boundary condition cells: there is one entry for the parent grid boundary cells and one entry for each of the child grid cells.



After a successful MODFLOW-LGR run, you will see multiple entries in the Output directory: Heads for the parent grid and Heads for each of the child grids, and likewise for Drawdown.



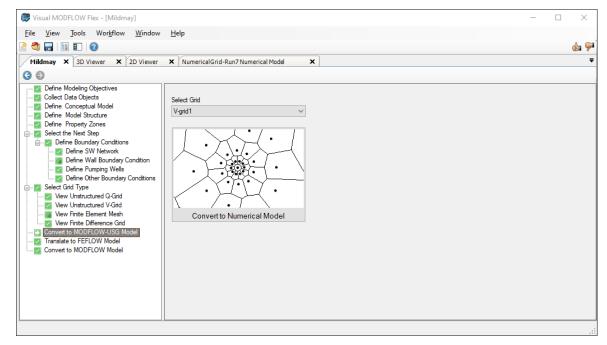
9.2 Converting to Unstructured Grid Numerical Model (MODFLOW-6/USG)

Quick Overview

Instructions	Create an Unstructured Grid numerical model (MODFLOW-6/USG) by populating the selected grid with data from the conceptual model
Pre-requisites:	An Unstructured <u>V-Grid</u> or <u>Q-Grid</u> has been created.
Result:	A numerical model is generated and added to the Model Explorer tree. The numerical model workflow will appear.
Next Steps:	Numerical Modeling Workflow (Unstructured)

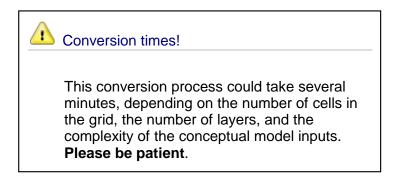
Once you have the conceptual model designed and at least one UnStructured V-Grid or Q-Grid, you are ready to populate this grid with the conceptual data.

Proceed to the "Convert to MODFLOW-USG Model" step in the Conceptual Model workflow; this is shown in the display below.

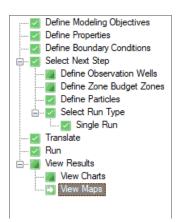


The Select Grid combo box will list all the Unstructured grids you have created for your project

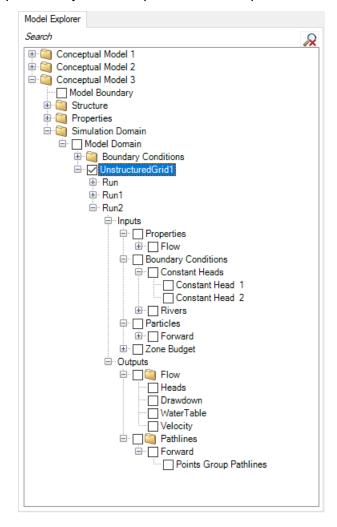
Select the grid you wish to use ,and click on the "Convert to Numerical Model" button.



After the conversion is complete, a new numerical model workflow window will appear which includes the steps for viewing and editing the unstructured grid numerical model.



During the conversion, a "Run" node will be added to the Model Explorer under the UnStructured grid that you selected. This Model Explorer tree will be populated with all the inputs from your conceptual model: Properties, Boundary Conditions, Wells, etc.



When the conversion is complete, you can click on the S Next button on the workflow toolbar, which will take you to the View/Edit Properties. You can then proceed through the Unstructured grid numerical model workflow.

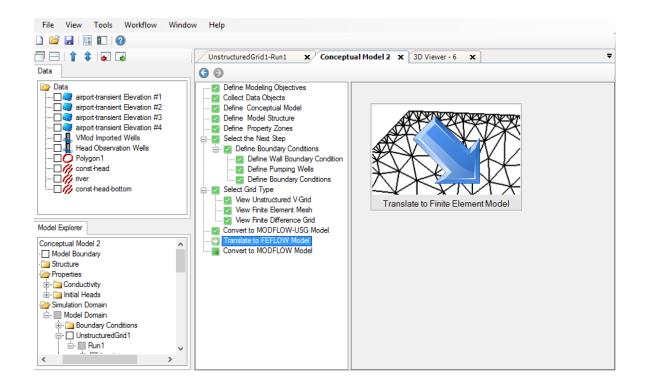
9.3 Converting to FEFLOW

Quick Overview

Instructions	Create a FEFLOW .FEM file by populating the selected mesh with data from the conceptual model
Pre-requisites:	A Finite Element Mesh has been created
Result:	A FEFLOW .FEM file (.ASCII) is generated.
Next Steps:	Open this project file in FEFLOW v.5.4 or later

Once you have the conceptual model designed and at least one finite element mesh, you are ready to populate this mesh with the conceptual data.

Proceed to the "Translate to Finite Element Model" step in the Conceptual Model workflow; this is shown in the display below.



Translate to Finite Element Model Options

Click on the Translate to Finite Element model button, and the following dialog will appear. (Alternatively, you can select the Conceptual model folder in the Model Explorer tree, and select Translate to Finite Element Model... from the pop-up menu.)

Project Description		
mmaytesta		
Finite Element Mesh		
FiniteElementMesh1		•
Output name		
C:\Users\Administrator\Desktop\VMC	ODFlex-Projects\NumericalModels\FEFLOW\FiniteEleme	n
ranslation Log file		
C:\Users\Administrator\Desktop\VMC	ODFlex-Projects\NumericalModels\FEFLOW\FiniteEleme	ntMes
Problem Class		
Separate flow problem		-
imulation Type		
Steady-state		-
Flow Type		
Saturated media (groundwater)		-
Franslation Format		
FEFLOW (v.5.404) ASCII FEM file		-
Start Date		
10/ 5/2005		
Start Time		
12:00:00 AM		
teady-State Simulation Time [day]		-

Project Description

A brief description of the project. By default, this is the name of the current Visual MODFLOW Flex project.

Finite Element Mesh

Select the desired finite element mesh from the combo box to use for model translation.

Output Name

Click the _____ button and specify the output name and directory for the *.FEM file that is created during translation.

The .FEM file is an ASCII file containing information on the problem class and model properties. This file is required for importing your model into FEFLOW.

The default file name is "Project_name.FEM" and the default directory on your computer is [Project Folder]\Numerical Models.

Translation Log File

When a numerical model is translated in Visual MODFLOW Flex, a log file is automatically generated and saved on your computer. By default the log file name is [Project_Name].LOG and the directory is [Project Name]\Numerical Models.

Click the ____ button to specify a new file name and directory.

Problem Class

Currently, Visual MODFLOW Flex only supports the separate flow problem class.

Simulation Type

Select Steady State or Transient from the combo box.

If the Steady State option is selected, Visual MODFLOW Flex will prepare the data set for a steady-state flow simulation, and will automatically use the data from the first stress period of each boundary condition and pumping well defined in your conceptual model.

If the Transient Flow option is selected, Visual MODFLOW Flex will automatically merge all the different time period data defined for each pumping well and boundary condition into the stress period format required by FEFLOW.

Flow Type

Select the flow type of the problem class. Choose from the following options: Saturated media (groundwater), unsaturated media, Unsaturated steady-state linearized Richards equation.

Translation Format

The output .FEM file generated by Visual MODFLOW Flex during translation is currently compatible with FEFLOW v.5.3.11 or later.

Start Date

The default start date is the date specified in the conceptual model settings. The Start Date of the model is the date corresponding to the beginning of the simulation. This date is relevant only for transient flow simulations where recorded field data may be used for defining time schedules for selected boundary conditions.

Start Time

Specify the simulation start time. The Start Time of the model is the time corresponding to the beginning of the simulation. This time is relevant only for transient flow simulations where recorded data may be imported for defining time schedules for selected boundary conditions.

Steady-State Simulation Time

A steady state simulation time is required for Steady State Flow simulation. This parameter is not used if you have selected Transient Flow. Although the simulation will always be run to the same equilibrium solution in Steady State, the total amount of water passing through boundary conditions (i.e. the cumulative value of the solution) depends on the amount of time simulated.

Name	Translate	FEFLOW Conditions		
Recharge boundary				
Recharge 1		Material: In/Out Flow	-	
Well boundary				
^o umpingWell1	V	BC: 4th kind	_	
charge and Evapotranspiratio	on Options			
charge and Evapotranspiratio Recharge	on Options			
		erty on top		
Recharge	T(-) flow prop			
Recharge Translate as IN(+)/OU	T(-) flow prop			
Recharge Translate as IN(+)/OU Translate Recharge to	T(-) flow prop 2nd type bo	undary condition		

The Packages frame contains a list of existing boundary conditions for the conceptual model being translated. Here you can include/exclude boundary conditions by selecting the

appropriate check box in the Translate column. The corresponding FEFLOW condition type is listed for each boundary condition under the FEFLOW Conditions column.

You can also select how Recharge and Evapotranspiration should be represented: As Flow Properties or as Type2 Boundary Condition.

Click the [Next] button to initiate the model translation. During translation, output details are displayed in the translation log. Once finished, click the [Finish] button to exit the translation wizard.

10 Numerical Modeling Workflow - Finite Difference Grids

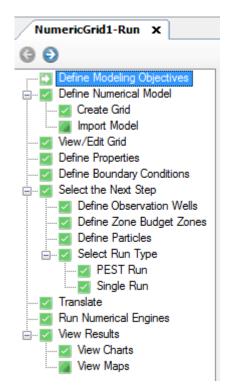
This chapter presents information on editing data in a numerical model workflow for regular grids; the numerical model can originate from:

- Importing a Visual MODFLOW Classic or MODFLOW project, or
- Executing a Conceptual to Numerical Model conversion

The numerical modeling workflow provides the tools for building the numerical model (properties and boundaries assigned to grid cells), running the MODFLOW engines, and analyzing the results. For information on editing data in an unstructured grid, see the related section on the <u>numerical model workflow for unstructured grids</u>.

The following sections are covered:

- 1. Define Modeling Objectives
- 2. <u>Define/Edit Grid</u> (if importing or creating a new numerical model)
- 3. <u>View/Edit Properties</u> (geometry and parameter edits)
- 4. <u>View/Edit Boundary Conditions</u> (constant heads, drains, pumping wells, recharge, etc.)
- 5. Define Observation Wells
- 6. Define Zone Budget Zones
- 7. Define Particles
- 8. Translation
- 9. Run Numerical Engines
- 10. View Results
 - <u>Contours and Color Floods</u>
 - <u>Charts</u>



10.1 Define Objectives

The first step in the workflow for developing and running numerical models in Visual MODFLOW Flex is to define the modeling objectives. This entails selecting the desired flow and transport simulation options. The selected combination of flow options (e.g. saturated

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groundwater flow) and transport options (e.g. reaction and sorption models) will narrow the list of available flow and transport engines and generate associated input variables (including units and default values). The purpose of this step is to develop the necessary inputs required to build the model based on your understanding of the relevant physical processes present within the study area.

The numerical workflow supports the following engines:

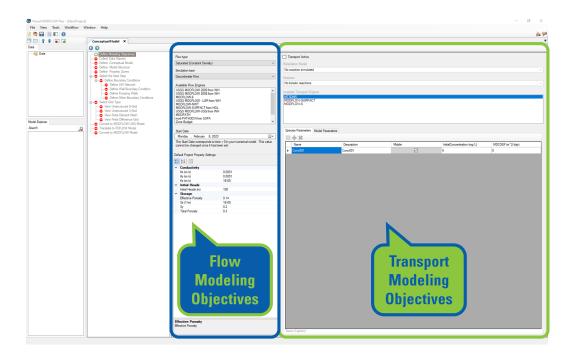
Flow Transport Utilities ZONEBUDGET • MODFLOW-2000 MT3DMS MODPATH MODFLOW-2005 RT3D • MOD-PATH3DU³ MODFLOW-NWT PEST MODFLOW-LGR none none ZONEBUDGET-6 • MODFLOW-6 • MODFLOW-6 • MODFLOW-• MODFLOW- MODPATH SURFACT¹ SURFACT¹ ZONEBUDGET SEAWAT² • SEAWAT² MODPATH

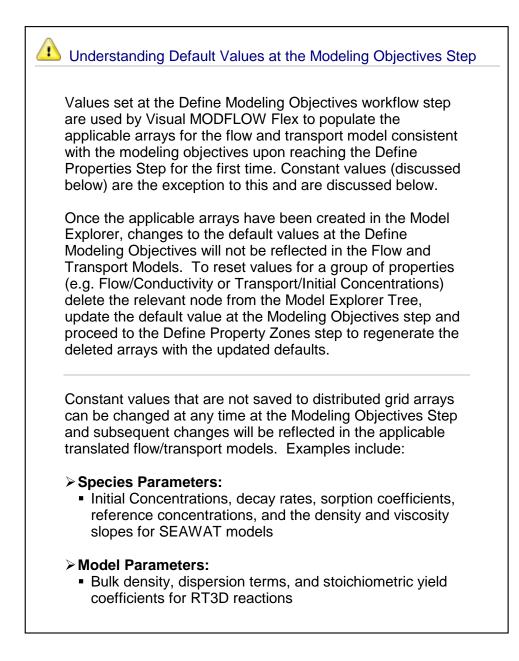
Engines supported in Visual MODFLOW Flex

Notes:

1 - MODFLOW-SURFACT is a commercial groundwater modeling engine that supports coupled groundwater flow and transport simulations.

2 - SEAWAT is a coupled variable density groundwater flow and transport model
3 - MOD-PATH3DU is a particle-tracking algorithm developed by a collaboration between
S.S. Papadopulos & Associates (SSPA) and the University of Waterloo. It is not installed
directly with Visual MODFLOW Flex and must be downloaded and installed separately
from the mod-PATH3DU website.





Flow Objectives

Under the left panel of Define Modeling Objectives, you can specify a Start Date for the project. Pumping well data and calibration data (head and concentration observation wells) are entered and save as absolute (calendar) dates. Therefore, it is important to choose a relevant start date at this step that coincides with the start time of your simulation.

Flow and Simulation Type

There are several flow condition options available for flow modeling in the numerical workflow:

Flow Engines and Modeling Objectives Supported in Visual MODFLOW Flex

Flow Type	Satur Flo		Vari	ably	Satura	ated F	low ¹					
Simulatio n	Consta nt	Variab le	Gro	undw	ater	Vapo	r Flow	Zone	MODPAT	MOD- PATH3D	Transpor	PEST
Туре	Density	Densit y	UZF	V	BC	V	BC	Budget	н	H U		
Engines												
MF- 2000	\checkmark							$\mathbf{\nabla}$	\checkmark	\checkmark	\checkmark	V
MF- 2005	\checkmark								\checkmark		\checkmark	V
MF- NWT			V						\checkmark		\checkmark	V
MF- LGR												
SEAWA T		V									SEAWAT	
MF- SURFA CT	A			V	V	V	V		V		MF- SURFAC T	
MF-6	V										MF-6	

Notes:

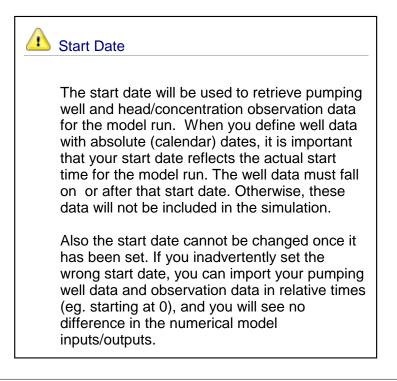
1 - Abbreviations for variably saturated flow processes in the Vadose Zone:

UZF = unsaturated zone flow package is based on 1-D unsaturated flow of a diffusion wave pseudo soil

V = Van Genuchten relative permeability and saturation relationship

BC = Brooks-Corey relative permeability and saturation relationship

Under Property Settings, you can modify the default flow parameters.



Start Date

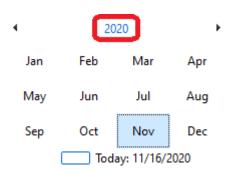
The model start date for this exercise should be set to 1/1/2000. Visual MODFLOW Flex uses a standard Windows date picker; a few tips are shown below on how to use this. Click on the button shown below, to load the Windows date picker.

🐯 Visual MODFLOW Flex - [Exercise]						- 0 ×
File View Tools Workflow W	/indow Help					
2 🎒 🔚 🗄 🗊 🕗						
🗇 🗁 l 🏦 🌲 🗛 👘 👘	Conceptual Model X					•
Data	G Ð					
	Define Modeling Objectives Collect Data Objects	Row type	Transport Active			
		Saturated (Constant Density) \lor	Retardation Model			
	Contract Define Property Zones	Simulation type	No sorption simulated			~
	Select the Next Step	Groundwater Flow \vee	Reaction			
	Define Boundary Conditions Define Wall Boundary Condition	Available Flow Engines	No kinetic reactions			×
	Define Pumping Wells Define Boundary Conditions	USGS MODFLOW 2000 from WH USGS MODFLOW 2005 from WH	Available Transport Engines			
	Select Grid Type View Unstructured V-Grid	USGS MODFLOW-LGR from WH MODFLOW-NWT	MT3DMS MODFLOW-SURFACT			
	View Finite Element Mesh	MODFLOW-SURFACT from HGL ZONFBUDGET				
	Wew Finite Difference Grid Convert to MODFLOW-USG Model	MODPATH				
	Convert to MODFLOW-USG Model Translate to FEFLOW Model					
Model Explorer	Convert to MODFLOW Model					
Search 🔗		Start Date	Species Parameters Model P	arameters		
		Tuesday , July 11, 2017 🗐 🔻	+ X			
		The Start Date corresponds to time = 0 in your numerical model. This value cannot be changed once it has been set.	Name	Description	Mobile	InitialConcentration (mg/L)
		Default Project Property Settings	Conc001	Conc001		0
		21 21 0				
		Kx (m/s) 0.0001				
		Ky (m/s) 0.0001 Kz (m/s) 1E-05				
		✓ Initial Heads				
		Initial Heads (m) 100 Storage				
		Ss (1/m) 1E-05				
		Sy 0.2 v				
		Initial Heads (m) Initial Heads				
		insui ricula	Name (Caption)			
	L					

The standard Windows calendar will appear. Click on the month in the header (as shown below):

•	- (Nove	ember	2020		×		
Sun	Mon	Tue	Wed	Thu	Fri	Sat		
25	26	27	28	29	30	31		
1	2	3	4	5	6	7		
8	9	10	11	12	13	14		
15	16	17	18	19	20	21		
22	23	24	25	26	27	28		
29	30	1	2	3	4	5		
	Today: 11/16/2020							

All months for the current year will appear as shown below. Click on the year in the header:



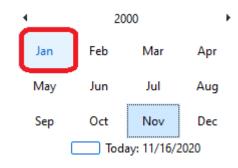
A range of years will then appear as shown below. Click on the range of years in the header:



A list of years for the previous decade will appear. You can then use the < or > buttons to change the year. Once you have reached the desired year (2000 for this example), select this on the calendar as shown below:



A list of months will then appear for that year. Select January for this example, as shown below.



Finally, select "1" from the calendar as shown below:

4			•						
Sun	Mon	Tue	Wed	Thu	Fri	Sat			
26	27	28	29	30	31	1			
2	3	4	5	6	7	8			
9	10	11	12	13	14	15			
16	17	18	19	20	21	22			
23	24	25	26	27	28	29			
30	31	1	2	3	4	5			
	Today: 11/16/2020								

The selected date will then appear for the Start Date.

Transport Objectives

The transport objectives are defined on the right panel of the Define Modeling Objectives window. When you select the "Transport Active" check box at the top of the screen, then the options can be defined as explained and shown below.

Retardation Model

Transport engine retardation model options are currently supported in Visual MODFLOW Flex as follows:

Description	MT3 DMS	RT 3D	SEA WAT	MF-6	SURF ACT
No Sorption		\checkmark			\checkmark
Linear sorption (equilibrium controlled)	\checkmark		$\mathbf{\nabla}$		V
Freundlich (equilibrium- controlled)	\checkmark				
Langmuir (equilibrium-controlled)		$\mathbf{\Sigma}$			
First order kinetic sorption (non- equilibrium)	V				
Dual-domain mass-transfer without sorption	\checkmark				V
Dual-domain mass-transfer with linear sorption in mobile domain	<u> </u>			V	V
Dual-Domain with Complex Sorption Options					
Triple-Domain with Complex Sorption Options					

Description	MT3 DMS	RT 3D	SEA WAT	MF-6	SURF ACT
Quadruple-Domain with Complex Sorption Options					
Dual-domain mass-transfer (with the same linear sorption in mobile and immobile domains)					V
Dual-domain mass-transfer (with different linear sorption in mobile and immobile domains)					V
Dual-domain mass-transfer with nonlinear sorption in mobile domain					V
Dual-domain mass-transfer (with the same nonlinear sorption in mobile and immobile domains)					V
Dual-domain mass-transfer (with different nonlinear sorption in mobile and immobile domains)					V

Reaction

Transport engine reaction model options are currently supported in Visual MODFLOW Flex as follows:

Description	MT3 DMS	RT 3D	SEA WAT	MF-6	SURF ACT ¹
No kinetic reactions					\checkmark
First-order irreversible decay					
Zeroth-order irreversible decay					
Complex Model Reactions ²					
Instantaneous aerobic degradation of of BTEX		\checkmark			
Six-Species, First-Order, Rate- Limited, BTEX Degradation using Sequential Electron Acceptors		V			
Rate-Limited Sorption		\checkmark			
Double-Monod Model		V			

Description	MT3 DMS	RT 3D	SEA WAT	MF-6	SURF ACT ¹
Sequential First-Order Decay		\checkmark			
Aerobic/Anaerobic PCE/TCE Dechlorination					

Notes:

1 - MODFLOW-SURFACT supports additional reactions listed in the table above; however, these are not fully supported in the current version of Visual MODFLOW Flex.

2 - Complex Reactions available for MODFLOW-6 allow for different reaction models (no kinetic reactions, first-order, and zero order decay) to be independently specified for each species and for each (mobile/immobile domain) in the aqueous and sorbed phases. Complex model reactions are only compatible with the three available complex sorption options (i.e. dual-domain, triple-domain, and quadruple-domain).



RT3D assumes specific default species for each associated reaction modules. Selecting a reaction module specific to RT3D will reset the species list and all associated species and model parameters

The selections you make for Sorption and Reaction options will determine what parameters you need to define for your model. Default values can be defined in the "Species Parameters" and "Model Parameter" tabs. After the model is created, you can define additional zonation for Transport Properties at the "Define Properties" step. Detailed information regarding these parameters can be found in the MT3DMS, RT3D, SEAWAT, SURFACT, and MODFLOW-6 User Manuals (please see the <u>references</u> section).

The New Species and Delete Species buttons allow you to add and remove species to your Transport simulation. This option is available only for certain transport engines.

When you Species Parameter tab is selected, use the add button (*) to add a new species, or use the remove button (*) to remove the selected species.

Please Note: the remove button will remove the *last* species in the list.

The reaction model parameters window is shown below. For more information, see the individual sections describing <u>Species Parameters</u> and <u>Model Parameters</u>.

\checkmark	Transport Active					
Ret	ardation Model					
N	o sorption simulated					~
Rea	action					
N	o kinetic reactions					~
Ava	ailable Transport Engine:	3				
M	T3DMS	-				
M	DDFLOW-SURFACT					
S	pecies Parameters Mo	del Parameters				
Γ	Name	Designation	Description	Value		Units
	IRCTOP	IRCTOP	How should reaction	By cell	\sim	
	IGETSC	IGETSC	Should sorbed or imm	No	\sim	

When you are finished, click 📀 (Next Step) to proceed.

10.1.1 Project Property Settings (Flow)

The default flow parameters are set in project property settings affecting can are set in the Default Project Property Settings area which is divided into four groups: Conductivity, Initial Heads, Storage, and Unsaturated Zone (which will only show if variably saturated flow using the MODFLOW UZF model is selected as a flow modeling objective.

~	Conductivity				
	Kx (m/s)	0.0001			
	Ky (m/s)	0.0001			
	Kz (m/s)	1E-05			
~	Initial Heads				
	Initial Heads (m)	100			
~	Storage				
	Effective Porosity	0.14			
	Ss (1/m)	1E-05			
	Sy	0.2			
	Total Porosity	0.3			
~	Unsaturated Zone Properties				
	EPS	3.5			
	THTi	0.3			
	THTs	0.3			
-	fective Porosity				

Values will serve as the defaults for the model when the grid arrays in the model explorer are first populated. Note that once the grid arrays in the model explorer have been populated, changing the default values will not have any effect on the model. Changes can be made at the <u>Define Properties</u> step or to reset the values of a group back to defaults, delete the applicable node on the model explorer, update the default values as desired at the Modeling Objectives, and proceed to the Define Properties step to regenerate the deleted arrays.

These properties can be changed for all new projects on the <u>Model Defaults</u> tab of the Project Settings.

Conductivity

- Kx Hydraulic conductivity in the direction of the model X-axis, specified in conductivity units [L/T]
- **Ky** Hydraulic conductivity in the direction of the model Y-axis, specified in conductivity units [L/T]
- Kz Hydraulic conductivity in the direction of the model Z-axis, specified in conductivity units [L/T]

Storage

- Effective Porosity, [-]
- Ss specific storage, [-]
- Sy specific yield, [-]
- Total Porosity, [-]

Initial Heads

• Initial heads, [L]

Unsaturated Zone Properties - UZF package only

- EPS Brooks-Corey exponent ε, [-]
- **THTi** initial water saturation θ_i , [-]
- **THTs** residual water saturation θ_r , [-]

10.1.2 Species Parameters

The Species Parameters include the Sorption and Reaction parameters used by the selected transport settings. The available parameters will depend on what sorption and reaction settings you selected in the Modeling Objectives workflow step. The parameters presented in the Species Parameters Database window are from the parameters listed in the Species Parameters Tab in the Modeling Objectives workflow step.

If no sorption or reactions are selected in the current transport variant, then no sorption or reaction parameters are required for the simulation, and there will not be an option for "Species Parameters" at the Define Properties workflow step.

The parameters are described by <u>retardation model</u> and <u>reaction model</u> below and for the special case of <u>variable density flow</u> (SEAWAT) models.

General

The following species parameters will be available for any model where transport is a defined modeling objective:

- Name: the short name of each species to be modeled (e.g. TCE for trichloroethylene)
- **Description**: a more descriptive name for each species to be modeled (e.g. trichloroethylene when modeling TCE)
- Initial Concentration: the concentration of each species throughout the model domain at the start of the simulation [default=0]. See <u>Theory</u>.
- Diffusion Coefficient: the Fickian diffusion constant for each species. See <u>Theory</u>.

Retardation Model - Species Parameters

The list of parameters required for each species based on each retardation model is provided below, associated base units are provided in square brackets [], where L signifies length (e.g. meters, feet), M signifies mass (e.g. kilograms, pounds), and T signifies time (e.g. seconds, days, years).

A tabulation of which retardation model is supported by each of the transport engines is provided in the <u>Define Modeling Objectives</u> workflow step. For more detailed documentation on each of the retardation model parameters, please refer to the documentation of the relevant transport engine (i.e. <u>MT3DMS</u>, <u>RT3D</u>, <u>SEAWAT</u>, <u>MODFLOW-SURFACT</u>, or <u>MODFLOW-6</u>).

Linear Isotherm (equilibrium controlled)

• Kd is the distribution coefficient [1/(M/L³)]

Freundlich (equilibrium-controlled)

- **Kf** is the Freundlich constant $[1/(M/L^3)^a]$
- a is the Freundlich exponent [-]

Langmuir (equilibrium-controlled)

- KI is the Langmuir is constant [1/(M/L³)]
- S is the total concentration of sorption sites available [-]

First order kinetic sorption (non-equilibrium)

- Kd is the distribution coefficient [1/(M/L³)]
- K_mass is the first-order kinetic mass transfer coefficient [1/T]

Dual-domain mass-transfer without sorption

- SCONCIM is the initial concentration in the distribution coefficient [1/(M/L³)]
- K_mass is the first-order kinetic mass transfer coefficient [1/T]

Dual-domain mass-transfer with linear sorption in mobile domain

- SCONCIM is the initial concentration in the immobile domain [M/L3]
- Kd is the distribution coefficient for the mobile domain [1/(M/L³)]
- K_mass is the first-order kinetic mass transfer coefficient [1/T]

Dual Domain with Complex Sorption

- SCONCIM1 is the initial concentration in the (first) immobile domain [M/L3]
- Kd is the linear distribution coefficient for the mobile domain [1/(M/L³)]
- KI is the Langmuir is constant for the mobile domain [1/(M/L³)]
- S is the total concentration of sorption sites available in the mobile domain [-]
- Kf is the Freundlich constant [1/(M/L³)^a]

- a is the Freundlich exponent [-]
- Kd_Im1 is the linear distribution coefficient for the (first) immobile domain [1/(M/L3)]
- K_mass1 is the first-order kinetic mass transfer coefficient between the mobile domain and the (first) immobile domain [1/T]

Note that this retardation model includes all available species parameters for speciesdependent sorption and mass-transfer between the mobile and immobile domain available in MODFLOW-6. In this case, the translation settings should be used to specify which processes are included in the model on a per-species basis. For more information, please see the property zones <u>Theory</u> section, including a description of <u>incompatible and mutually</u> <u>exclusive</u> parameters.

Triple Domain with Complex Sorption

- SCONCIM1 is the initial concentration in the (first) immobile domain [M/L³]
- SCONCIM2 is the initial concentration in the (second) immobile domain [M/L³]
- Kd is the linear distribution coefficient for the mobile domain [1/(M/L³)]
- KI is the Langmuir is constant for the mobile domain [1/(M/L³)]
- S is the total concentration of sorption sites available in the mobile domain [-]
- Kf is the Freundlich constant [1/(M/L³)^a]
- a is the Freundlich exponent [-]
- Kd_Im1 is the linear distribution coefficient for the (first) immobile domain [1/(M/L³)]
- K_mass1 is the first-order kinetic mass transfer coefficient between the mobile domain and the (first) immobile domain [1/T]
- Kd_Im2 is the linear distribution coefficient for the (second) immobile domain [1/(M/L³)]
- K_mass2 is the first-order kinetic mass transfer coefficient between the mobile domain and the (second) immobile domain [1/T]

Note that this retardation model includes all available species parameters for speciesdependent sorption and mass-transfer between the mobile and immobile domains available in MODFLOW-6. In this case, the translation settings should be used to specify which processes are included in the model on a per-species basis. For more information, please see the property zones <u>Theory</u> section, including a description of <u>incompatible and mutually</u> <u>exclusive</u> parameters.

Quadruple with Complex Sorption

- SCONCIM1 is the initial concentration in the (first) immobile domain [M/L3]
- SCONCIM2 is the initial concentration in the (second) immobile domain [M/L³]
- SCONCIM3 is the initial concentration in the (third) immobile domain [M/L3]
- Kd is the linear distribution coefficient for the mobile domain [1/(M/L³)]
- KI is the Langmuir is constant for the mobile domain [1/(M/L³)]
- S is the total concentration of sorption sites available in the mobile domain [-]
- Kf is the Freundlich constant [1/(M/L³)^a]
- **a** is the Freundlich exponent [-]
- Kd_Im1 is the linear distribution coefficient for the (first) immobile domain [1/(M/L³)]
- **K_mass1** is the first-order kinetic mass transfer coefficient between the mobile domain and the (first) immobile domain [1/T]
- Kd_Im2 is the linear distribution coefficient for the (second) immobile domain [1/(M/L3)]
- **K_mass2** is the first-order kinetic mass transfer coefficient between the mobile domain and the (second) immobile domain [1/T]
- Kd_Im3 is the linear distribution coefficient for the (third) immobile domain [1/(M/L³)]
- K_mass3 is the first-order kinetic mass transfer coefficient between the mobile domain and the (third) immobile domain [1/T]

Note that this retardation model includes all available species parameters for speciesdependent sorption and mass-transfer between the mobile and immobile domains available in MODFLOW-6. In this case, the translation settings should be used to specify which processes are included in the model on a per-species basis. For more information, please see the property zones <u>Theory</u> section, including a description of <u>incompatible and mutually</u> <u>exclusive</u> parameters.

Dual-domain mass-transfer with the same linear sorption in mobile and immobile domains

• SCONCIM is the initial concentration in the immobile domain [M/L³]

- Kd is the distribution coefficient for both the mobile and immobile domain [1/(M/L³)]
- K_mass is the first-order kinetic mass transfer coefficient [1/T]

Dual-domain mass-transfer with different linear sorption in mobile and immobile domains

- SCONCIM is the initial concentration in the immobile domain [M/L³]
- Kd is the distribution coefficient for the mobile domain [1/(M/L³)]
- K_mass is the first-order kinetic mass transfer coefficient [1/T]
- KdIm is the distribution coefficient for the immobile domain [1/(M/L³)]

Dual-domain mass-transfer with nonlinear sorption in mobile domain

- SCONCIM is the initial concentration in the immobile domain [M/L³]
- Kf is the Freundlich constant for the mobile domain $[1/(M/L^3)^a]$
- a is the Freundlich exponent for the mobile domain [-]
- K_mass is the first-order kinetic mass transfer coefficient [1/T]

Dual-domain mass-transfer with the same nonlinear sorption in mobile and immobile domains

- SCONCIM is the initial concentration in the immobile domain [M/L3]
- Kf is the Freundlich constant for both the mobile and immobile domain $[1/(M/L^3)^a]$
- a is the Freundlich exponent for both the mobile and immobile domain [-]
- **K_mass** is the first-order kinetic mass transfer coefficient [1/T]

Dual-domain mass-transfer (with different linear sorption in mobile and immobile domains)

- SCONCIM is the initial concentration in the immobile domain [M/L3]
- Kf is the Freundlich constant for the mobile domain [1/(M/L³)^a]
- **a** is the Freundlich exponent for the mobile domain [-]
- K_mass is the first-order kinetic mass transfer coefficient [1/T]
- Kflm is the Freundlich constant for the immobile domain [1/(M/L³)^{aim}]
- **aim** is the Freundlich exponent for the immobile domain [-]

Please Note: Immobile species must be at the bottom of the species list on the Transport Modeling Objectives; be sure to add these to the species list last.

Reaction Model - Species Parameters

The list of parameters required for each species based on each reaction model is provided below, associated base units are provided in square brackets [], where L signifies length (e.g. meters, feet), M signifies mass (e.g. kilograms, pounds), and T signifies time (e.g. seconds, days, years).

A tabulation of which reaction model is supported by each of the transport engines is provided in the <u>Define Modeling Objectives</u> workflow step. For more detailed documentation on each of the retardation model parameters, please refer to the documentation of the relevant transport engine (i.e. <u>MT3DMS</u>, <u>RT3D</u>, <u>SEAWAT</u>, <u>MODFLOW-6</u>, or <u>MODFLOW-SURFACT</u>).

Please Note: The RT3D reactions have specific default species for each of its associated reaction modules. Selecting a reaction module specific to RT3D will reset the species list and all associated species and model parameters.

First-Order Irreversible Decay

- **K_mobile** (or **K1**) is the first-order decay rate coefficient for dissolved constituents in both the mobile (and immobile domain, if applicable) [1/T]
- **K_sorbed** (or **K1_sorbed**) is the first-order decay rate coefficient for sorbed constituents in both the mobile (and immobile domain, if applicable) [1/T]
- **K1_im1** is the first-order decay rate coefficient for dissolved consitituents in the first immobile domain [1/T]
- K1_im1_sorbed is the first-order decay rate coefficient for sorbed consitituents in the first immobile domain [1/T]
- **K1_im2** is the first-order decay rate coefficient for dissolved consitituents in the second immobile domain [1/T]
- K1_im2_sorbed is the first-order decay rate coefficient for sorbed consitituents in the second immobile domain [1/T]
- **K1_im3** is the first-order decay rate coefficient for dissolved consitituents in the third immobile domain [1/T]
- K1_im3_sorbed is the first-order decay rate coefficient for sorbed consitituents in the third immobile domain [1/T]

Please Note: First-order decay rate coefficients can be derived from half-life values, which are more commonly available. Concentrations that follow first-order decay can be shown to change over time by the equation:

Zeroth-Order Irreversible Decay

- **K_mobile** (or **K0**) is the zeroth-order decay rate coefficient for dissolved constituents in both the mobile (and immobile domain, if applicable) [1/T]
- **K_sorbed** (or **K0_sorbed**) is the zeroth-order decay rate coefficient for sorbed constituents in both the mobile (and immobile domain, if applicable) [1/T]
- K0_im1 is the zeroth-order decay rate coefficient for dissolved consitiuents in the first immobile domain [1/T]
- K0_im1_sorbed is the zeroth-order decay rate coefficient for sorbed consitituents in the first immobile domain [1/T]
- K0_im2 is the zeroth-order decay rate coefficient for dissolved consitituents in the second immobile domain [1/T]
- K0_im2_sorbed is the zeroth-order decay rate coefficient for sorbed consitituents in the second immobile domain [1/T]
- K0_im3 is the zeroth-order decay rate coefficient for dissolved consitituents in the third immobile domain [1/T]
- K0_im3_sorbed is the zeroth-order decay rate coefficient for sorbed consitituents in the third immobile domain [1/T]

RT3D Reaction Modules

The RT3D engine was designed to simulate more complex reaction models involving the interaction of species concentrations through interdependent reactions. Visual MODFLOW Flex includes support for the six built-in reaction models that may be of interest in a large number of sites:

- Instantaneous aerobic degradation of of BTEX;
- Six-Species, First-Order, Rate-Limited, BTEX Degradation using Sequential Electron Acceptors;
- Rate-Limited Sorption;
- Double-Monod Model;
- · Sequential First-Order Decay; or
- Aerobic/Anaerobic PCE/TCE Dechlorination

Selecting any of these reaction models will reset the species listed at the Define Modeling Objectives step to a list of pre-defined species particular to the specified reaction model.

RT3D Decaying Source

• Source Decay Constant is the first-order decay rate coefficient for decaying sources [1/T]

RT3D uniquely supports specified "constant" concentration boundary conditions with a decaying source term. The source term is defined as:

 $C_i = C_{i,0} e^{-\lambda t}$

where:

 C_i is the concentration of the ith constituent at time t [M/L³]

 $C_{i,0}$ is the concentration of the ith constituent at the beginning of the stress period [M/L³]

 λ is the first-order source decay rate constant [1/T]

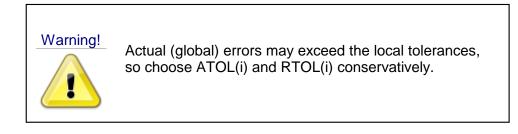
t is elapsed time since the beginning of the stress period [T]

RT3D Solution Parameters

The **Absolute Tolerance (ATOL)** and **Relative Tolerance (RTOL)** species parameters will be added for each species. These tolerance parameters are used by the differential equations solver in RT3D to control convergence errors while solving the applicable reaction model. Setting ATOL(i) = 0.0 results in a pure relative error test on Species i, while setting RTOL(i) = 0.0 results in a pure absolute error test on Species i. For practical problems, the following rules of thumb may be used to set ATOL and RTOL values:

- set RTOL(i) = 10-(m+1), where m is the desired number of significant digits for concentration output for species i (C_i)
- set ATOL(i) to a small value at which the absolute value of C_i is essentially insignificant (typically between 10⁻⁶ to 10⁻⁹)

Please Note: that RTOL > ATOL > 0



Variable Density Flow

The list of parameters required for a variable density flow model are presented below, associated base units are provided in square brackets [], where L signifies length (e.g.

meters, feet), M signifies mass (e.g. kilograms, pounds), T signifies time (e.g. seconds, days, years), and O signifies temperature (currently only degrees Celsius [°C] are supported, as these units are hard-coded into the governing equations implemented in SEAWAT). For more detailed information, see discussion on the <u>variable density</u> and <u>viscosity</u> packages.

- **Temperature**: this is a logical flag to select the species representing temperature. At most one species may be selected. This will link the selected temperature species to the viscosity package and change the concentration units to temperature. [-]
- Initial Concentration: same as above [see units item below]
- **CREF**: represents the reference concentration for the <u>density</u> and <u>viscosity</u> relationships for each species. [*see units item below*]
- Units: shows the project concentration units for all species [M/L³]; for the temperature species (if any) which will be shown in Θ, although currently only °C is supported].
- DRHODC (δρ/δC_i): the density versus concentration slope [-]; for the temperature species (if any), it represents δρ/δT [(M/L³)/T]
- DMUDC (δμ/δC_i): the dynamic viscosity versus concentration slope [L²/T]; for the temperature species (if any), it represents δμ/δT, if the linear-relationship option is selected [(M/L³)/T].
- **MDCOEFF:** species-specific diffusion coefficient [L²/T]. **Note**: this is only used if the multi-diffusion option is set to true in the DSP package advanced settings.

Please Note: If you are developing a *multi-species* variable-density model, the major density-controlling species (typically salt) should be Species 1. Furthermore, if you are also modeling temperature, temperature should be species number 2. Please refer to the SEAWAT v4 Manual by Langevin et al (2007) for more details about the implementation of density-dependent solute and thermal flow and transport in SEAWAT.

10.1.3 Model Parameters

Model parameters consist of material properties relevant to fate and transport modeling associated with the geologic units that are independent of the constituent species to be modeled. The specific model parameters required as part of each simulation are defined by the <u>retardation model</u> and <u>reaction model</u>.

General Model Parameters:

IRCTOP

IRCTOP is an integer flag indicating how reaction variables are entered:

- By Cell (IRCTOP=2) [Default] all reaction variables are specified as 3-D arrays on a cell-by-cell basis.
- By Layer (IRCTOP=0) all reaction variables are specified as a 1-D array with each value in the array corresponding to a single layer. This option is mainly for retaining compatibility with the previous versions of MT3D.

IRCTOP does not apply in MODFLOW-6 simulations

IGETSC

IGETSC is an integer flag indicating whether the initial concentration for the non-equilibrium sorbed or immobile phase of all species should be read when non-equilibrium sorption (ISOTHM = 4) or dual-domain mass transfer (ISOTHM = 5 or 6) is simulated. The flag is set by answering the question: *Should sorbed or immobile-phase concentrations be read?*

- No then IGETSC = 0 and the initial concentration for the sorbed or immobile phase is not read. By default, the sorbed phase is assumed to be in equilibrium with the dissolved phase (ISOTHM = 4), and the immobile domain is assumed to have zero concentration (ISOTHM = 5 or 6).
- Yes then IGETSC =1 and the initial concentration for the sorbed phase or immobile liquid phase of all species will be read, as applicable.

IGETSC does not apply in MODFLOW-6 simulations; initial concentrations are always read for dissolved solute concentrations in the mobile domain (and immobile domains as applicable) and only non-kinetic/equilibrium sorption models are supported.

Retardation Model - Model Parameters

Bulk Density (RHOB)

Soil Bulk Density is the dry mass of the soil divide by the volume of the soil and is used to calculate <u>retardation</u> factors. The default soil bulk density value for any new model created is 1700 kg/m³. If no sorption method is selected, in the current transport variant, then no bulk density values are required for the simulation, and all of the options in the left-hand toolbar will be disabled. For most transport engines (MT3D-MS, RT3D, SEAWAT, and SURFACT), a single bulk density is specified per model cell for the mobile and immobile domains. However, for MODFLOW-6, the dry bulk density may be defined per model cell separately for the mobile domain (*RHOB*) and for each immobile domain (*RhoIm1, RhoIm2, RhoIm3*), as applicable. The dry bulk density of the immobile domain is used to calculate the mass balance terms for decay of sorbed constituents in each respective immobile domain. For more information, please see the technical documentation for the MODFLOW-6 Groundwater Transport Model by Langevin, et al (2022).

- **RHOB** is the dry bulk density of the soil [M/L³]. the default soil bulk density value for any new model created is 1700 kg/m³
- **Rhobim** (or **Rhoim1**) is the dry bulk density of the soil in the first immobile domain $[M/L^3]$
- Rholm2 is the dry bulk density of the soil in the second immobile domain [M/L³]
- Rholm3 is the dry bulk density of the soil in the third immobile domain [M/L³]

Immobile Domain Porosity (Philm)

Immobile domain porosity is used to calculate the mass balance of constituents in the immobile domain.

- Philm (or Philm1) is porosity of the (first) immobile domain as the volume of the (first) immobile domain pore space per total volume [L³/L³] → [-]
- Philm2 is porosity of the second immobile domain as the volume of the second immobile domain pore space per total volume [L³/L³] → [-]
- **Philm3** is porosity of the third immobile domain as the volume of the second immobile domain pore space per total volume $[L^3/L^3] \rightarrow [-]$
- **PhiF** is the fraction of the mobile domain relative to the total volume $[L^3/L^3] \rightarrow [-]$

For more information, please see the property zones <u>Theory</u> section.

Reaction Model/Modules - Model Parameters

The reaction modules associated with RT3D may require model parameter values and settings to be selected at the Define Modeling Objectives workflow step, these include:

- Instantaneous aerobic degradation of BTEX [IREACT=1];
- <u>Six-Species</u>, First-Order, Rate-Limited, BTEX Degradation using Sequential Electron Acceptors [IREACT=3];
- Rate-Limited Sorption [IREACT=4];
- Double-Monod Model [IREACT=5];
- Sequential First-Order Decay [IREACT=6]; and
- <u>Aerobic/Anaerobic PCE/TCE Dechlorination</u> [IREACT=7]

where IREACT is a flag in the RT3D RCT package file whose value determines which reaction module is active in the transport model run.Note that the developers of RT3D did not implement a reaction model for IREACT=2 (Clement, <u>2003</u>).

Please Note: yield values associated with several reaction modules in RT3D are defined on a mg/L basis. To be consistent the user must use mg/L units for all concentrations when using these reaction modules. See additional notes for each reaction module.

Instantaneous aerobic degradation of BTEX

Paramet er	Caption	Description	Default	Units	Constant / Spatially Variable	Node in Model Explorer
RC1	Y_O2/BT EX	Stoichiometric ratio of oxygen (consumed) to BTEX	3.14	[-]	Const	n/a

Paramet er	Caption	Description	Default	Units	Constant / Spatially Variable	Node in Model Explorer
						Stoichiomet ry

* Note: By changing the value of RC1 instantaneous reactions between any other chemicals can be simulated using this module

Six-Species, First-Order, Rate-Limited, BTEX Degradation using Sequential Electron Acceptors

Paramet er	Caption	Description	Default	Units	Constant / Spatially Variable	Node in Model Explorer
RC1	Cmax_Fe 2+	Maximum concentration of Fe2+	0	[M/L ³]	Const/Var	R3-
RC2	Cmax_C H4	Maximum concentration of CH4	0	[M/L ³]	Const/Var	3(Reduction Capacities)
RC3	K_02	Hydrocarbon decay rate via aerobic process	0	[1/T]	Const/Var	
RC4	K_NO3	Hydrocarbon decay rate via denitrification	0	[1/T]	Const/Var	
RC5	K_Fe3+	Hydrocarbon decay rate via iron reduction	0	[1/T]	Const/Var	R3-3(Rates)
RC6	K_SO4	Hydrocarbon decay rate via sulfate reduction	0	[1/T]	Const/Var	
RC7	K_CH4	Hydrocarbon decay rate via methanogenesis	0	[1/T]	Const/Var	
RC8	Ks_O2	Half-saturation constant for oxygen	0.5	[M/L ³]	Const/Var	
RC9	Ks_NO3	Half-saturation constant for nitrate	0.5	[M/L ³]	Const/Var	
RC10	Ks_Fe3+	Half-saturation constant for Fe3+	0.5	[M/L ³]	Const/Var	R3- 3(Saturation
RC11	Ks_SO4	Half-saturation constant for sulfate	0.5	[M/L ³]	Const/Var	s)
RC12	Ks_CH4	Half-saturation constant for methane	0.5	[M/L ³]	Const/Var	
RC13	Ki_O2	Inhibition coefficient for the oxygen reaction	0.01	[M/L ³]	Const/Var	
RC14	Ki_NO3	Inhibition coefficient for the nitrate reaction	0.01	[M/L ³]	Const/Var	R3- 3(Inhibitions
RC15	Ki_Fe3+	Inhibition coefficient for the Fe3+ reaction	10	[M/L ³]	Const/Var	
RC16	Ki_SO4	Inhibition coefficient for the sulfate reaction	0.01	[M/L ³]	Const/Var	
RC17	Y_O2/BT EX	Stoichiometric ratio of oxygen (consumed) to BTEX	3.14	[-]*	Const	n/a Stoichiomet
RC18	Y_NO3/B TEX	Stoichiometric ratio of nitrate (consumed) to BTEX	4.9	[-]*	Const	ry

Paramet er	Caption	Description	Default	Units	Constant / Spatially Variable	Node in Model Explorer
RC19	Y_Fe/BT EX	Stoichiometric ratio of Fe2+ (produced) to BTEX	21.8	[-]*	Const	
RC20	Y_SO4/B TEX	Stoichiometric ratio of sulfate (consumed) to BTEX	4.7	[-]*	Const	
RC21	Y_CH4/B TEX	Stoichiometric ratio of methane (produced) to BTEX	0.78	[-]*	Const	

* Note: Yield values are on a mg/L basis; to be consistent, the user must use mg/L units for all concentrations when using this reaction module

Rate-Limited Sorption

Paramet er	Caption	Description	Default	Units	Constant / Spatially Variable	Node in Model Explorer
RC1	K_mt	Mass-transfer rate coefficient	0	[1/T]	Const/Var	R3-
RC2	Kd	Linear partitioning coefficient (Kd)	1	[L ³ /M]	Const/Var	4(Sorption)

Double-Monod Model

Paramet er	Caption	Description	Default	Units	Constant / Spatially Variable	Node in Model Explorer
RC1	µ_m(w)	Specific utilization rate	0	[1/T]	Const/Var	R3-5(Rates)
RC2	Ks_d	Monod half-saturation constant for electron donor	0.5	[M/L ³]	Const/Var	R3- 5(Saturation
RC3	Ks_a	Monod half-saturation constant for electron acceptor	0.5	[M/L ³]	Const/Var	s)
RC4	Y_x/d	Biomass produced per unit of electron donor utilized	0	[-]	Const	n/a Stoichiomet
RC5	Y_a/d	Electron acceptor used per unit of electron donor utilized	0	[-]	Const	ry
RC6	K_decay	First-order bacterial death or decay rate	0	[1/T]	Const/Var	
RC7	K_attach	First-order bacterial attachment rate	0	[1/T]	Const/Var	R3-5(Rates)
RC8	K_detach	First-order bacterial detachment rate	0	[1/T]	Const/Var	

* **Note**: This reaction module describes a general double Monod model. By setting appropriate yield and kinetic rate constants, users can model many types of biological systems. Kinetic constants for an aerobic system are given in Clement et al. (<u>1998</u>), and for an anaerobic denitrifying system are given in Clement et al. (<u>1997</u>). Also see Taylor and Jaffe (<u>1990</u>); Hornberger et al. (<u>1992</u>); Zysset et al. (<u>1994</u>); and Reddy and Ford (<u>1996</u>).

Paramet er	Caption	Description	Default	Units	Constant / Spatially Variable	Node in Model Explorer
RC1	K_A	PCE first-order degradation rate	0	[1/T]	Const/Var	
RC2	K_B	TCE first-order degradation rate	0	[1/T]	Const/Var	P2 6(Potoo)
RC3	K_C	DCE first-order degradation rate	0	[1/T]	Const/Var	R3-6(Rates)
RC4	K_D	VC first-order degradation rate	0	[1/T]	Const/Var	
RC5	Y_tce/pc e	Yield coefficient, TCE/PCE	0.792	[-]*	Const	n/a
RC6	Y_dce/tc e	Yield coefficient, DCE/TCE	0.738	[-]*	Const	Stoichiomet ry
RC7	Y_vc/dce	Yield coefficient, VC/DCE	0.644	[-]*	Const	

Sequential First-Order Decay

* Note: Yield values are on a mg/L basis; to be consistent, the user must use mg/L units for all concentrations when using this reaction module

Aerobic/Anaerobic PCE/TCE Dechlorination

Paramet er	Caption	Description	Default	Units	Constant / Spatially Variable	Node in Model Explorer
RC1	Кр	Sequential (anaerobic) reaction rate for PCE	0	[1/T]	Const/Var	
RC2	Kt1	Sequential (anaerobic) reaction rate for TCE	0	[1/T]	Const/Var	
RC3	Kt2	Aerobic decay rate for TCE	0	[1/T]	Const/Var	
RC4	Kd1	Sequential (anaerobic) reaction rate for DCE	0	[1/T]	Const/Var	
RC5	Kd2	Aerobic decay rate for DCE	0	[1/T]	Const/Var	R3-7(Rates)
RC6	Kv1	Sequential (anaerobic) reaction rate for VC	0	[1/T]	Const/Var	
RC7	Kv2	Aerobic decay rate for VC	0	[1/T]	Const/Var	
RC8	Ke1	Sequential (anaerobic) reaction rate for ETH	0	[1/T]	Const/Var	
RC9	Ke2	Aerobic decay rate for ETH	0	[1/T]	Const/Var	

* Note: All the yield values are fixed internally; to be consistent, use mg/L units for all species concentrations.

10.1.4 Theory

The following sections present an overview of the property zone parameters required for flow and transport models in Visual MODFLOW Flex.

A steady-state groundwater flow model requires conductivity and initial heads property values for each active grid cell in order to run a flow simulation, while transient flow models also require storage properties for each active grid cell. Similarly, a transport model requires various model and species parameter values for each active grid cell in order to run a transport simulation. Upon creating a Visual MODFLOW Flex project, the default flow and transport parameter values are assigned to every grid cell in the model domain. This will ensure the model has the minimum data required to run a simulation. However, in most situations, the flow and transport properties will not be uniform throughout the entire model domain, and it will be necessary to assign different property values to different areas of the model.

Heterogeneous property values are supported by Visual MODFLOW Flex using either Constant Value Property Zones, or Distributed Value Property Zones. These two different approaches are described below.

Constant Value Property Zones

The Constant Value Property Zones approach is the most simple and straight-forward, and can be used for all model properties supported by Visual MODFLOW Flex. Different model properties are accommodated by grouping grid cells sharing the same property values into "property zones". Each property zone will (normally) contain a unique set of property values, and is represented by a different grid cell color.

The Constant Value Property Zones approach requires the development of a conceptual model, whereby each hydrostratigraphic unit of the model is assigned a uniform set of property values. For example, consider an aquifer where there is pumping test data and slug test data indicating a range of horizontal conductivity values from 1×10^{-4} cm/s to 5×10^{-4} cm/s at different locations within the aquifer. One conceptual approach would assign a uniform Kx and Ky value of 2.5×10^{-4} cm/s to the entire aquifer. This value would be adjusted up or down for calibration purposes within the range of values reported. If a reasonable calibration cannot be achieved using this conceptual model, it may be necessary to sub-divide this region into several zones to accommodate local irregularities in the flow pattern. However, almost all modeling textbooks strongly recommend starting out simple at first, getting as close a solution as possible, and then making the model more complex, if necessary.

Distributed Value Property Zones

The Distributed Value Property Zones approach is available for flow properties (conductivity, storage, and initial Heads), and most transport properties (e.g. initial concentrations, longitudinal dispersivity, sorption parameters). This approach is a little more complicated than the constant value property zone approach because it involves linking a property zone to one or more parameter distribution arrays containing data interpolated from scattered observation points. When a property zone is linked to a distribution array, the property values assigned to each grid cell within that zone are calculated by multiplying the zone parameter value with the corresponding value from the parameter distribution array, a bivariate

interpolation scheme is used to calculate the appropriate parameter value at the center of the model grid cell using the four nearest data nodes in the parameter distribution array.

Flow Properties

Conductivity

Hydraulic conductivity is a property of both the porous media and the groundwater (or other fluid) passing through the pore space due to a pressure gradient based on Darcy's Law, an empirical relationship that relates the fluid flux to hydraulic gradient, with the conductivity as a constant of proportionality. In general:

$$q = -Ki$$

where:

q is the groundwater flux [L/T]

K is the hydraulic conductivity [L/T]

i is the hydraulic gradient, which is the change in pressure head over a distance, given by $\delta h/\delta l$ over infinitesimal distances or by $\Delta h/\Delta l$ over finite distances

It should be noted that Darcy's Law is limited to conditions where flow is laminar (slow and viscous), which is applicable in most groundwater systems.

Darcy's Law can be extended to three dimensional cases as follows:

$$q_{i} = -K_{ij} \nabla h = -\begin{bmatrix} K_{xx} & K_{xy} & K_{xz} \\ K_{yx} & K_{yy} & K_{yz} \\ K_{zx} & K_{zy} & K_{zz} \end{bmatrix} \begin{bmatrix} \delta h / \delta x \\ \delta h / \delta y \\ \delta h / \delta z \end{bmatrix}$$

where:

i and *j* are the X, Y, or Z principal directions

 K_{ij} is the hydraulic conductivity tensor with individual terms for flow in the *i* direction due to a gradient in the *j* direction

In most versions of MODFLOW and as currently implemented in Flex, the off-diagonal terms of the K_{ij} tensor are assumed to be negligible and the equation reduces to:

$$q_i' = -K_{ij}' \nabla h = -\begin{bmatrix} K_x & 0 & 0\\ 0 & K_y & 0\\ 0 & 0 & K_z \end{bmatrix} \begin{bmatrix} \delta h / \delta x\\ \delta h / \delta y\\ \delta h / \delta z \end{bmatrix}$$

The conductivity parameters may be defined on a cell-by-cell basis using constant property values and/or distributed property values. When importing or <u>assigning</u> the conductivity property zones, Visual MODFLOW Flex will require valid data for Kx, Ky, and Kz.

- Kx is defined as the hydraulic conductivity along the X-axis direction
- Ky is defined as the hydraulic conductivity along the Y-axis direction
- Kz is defined as the hydraulic conductivity along the Z-axis direction

Anisotropy

The reason Visual MODFLOW Flex prompts for both Kx and Ky is because there are two options for defining the horizontal anisotropy of the Conductivity property zones:

- Anisotropy by layer
- Anisotropy as specified

Please Note: The anisotropy option is set in Translation settings. (see <u>Anisotropy</u> for more details).

If the 'Anisotropy by layer' option is used, the Kx value will determine the conductivity in the X-direction, and the specified horizontal anisotropy ratio (Ky/Kx) for each layer will be used to calculate the Ky value for each grid cell. Dy default, the horizontal anisotropy is set to 1.

If the 'Anisotropy as specified' option is used, the model will use the Kx and Ky values defined for each property zone.

Storage

Storage parameters are used in transient simulations, particle tracking, and solute transport:

- Specific Storage (Ss) is defined as the volume of water that a unit volume of aquifer releases from storage under a unit decline in hydraulic head due to aquifer compaction and water expansion. Visual MODFLOW Flex determines the primary storage coefficient (sf1) for MODFLOW based on the user defined Specific Storage parameter. The primary storage coefficient is calculated by Visual MODFLOW Flex to be equal to the specific storage multiplied by the layer thickness (Specific Storage x thickness = Primary storage coefficient). Specific Storage is is only used in transient simulations.
- Specific Yield (Sy) is known as the storage term for an unconfined aquifer. It is defined as the volume of water that an unconfined aquifer releases from storage per unit surface area per unit decline in the water table. For sand and gravel aquifers, specific yield is generally equal to the porosity. MODFLOW uses Ss or Sy depending on the layer type assigned by the user (please refer to "Layer Type Settings"). For an unconfined layer, MODFLOW uses Sy to determine storage volumes. For a confined layer, Ss is used. For a variable layer, MODFLOW will check the head value of the cell to determine if it is confined or not. If you do not have measured parameter values for Sc and Sy it is recommended that you refer to literature values as a default. Specific Yield is only used in transient simulations.

- Effective Porosity (Eff. Por) is the pore space through which flow actually occurs, and is used by the particle tracking algorithms (MODPATH/MOD-PATH3DU) to determine the average linear groundwater velocities for use in time-dependent capture zones and time markers along pathlines. This term is not used for MODFLOW simulations.
- Total Porosity (Tot. Por) is the percentage of the rock or soil that is void of material, and is used by MT3D/RT3D/SEAWAT (by default) to determine the chemical reaction coefficients, and for calculating the average linear groundwater flow velocity in the particle tracking solution schemes. A different porosity is used for MT3D/RT3D/SEAWAT than for particle tracking because the transport engines account for additional transport and reactive processes, such as dispersion. The total porosity term is not used for MODFLOW simulations.

These storage parameters may be defined on a cell-by-cell basis using constant property values and/or distributed property values. When importing or <u>assigning</u> the storage property zones, Visual MODFLOW Flex will require valid data for each of the above parameters.

Please Note: MODFLOW-SURFACT supports the time-varying material properties (TMP1) package (as an add-on) where flow properties such as conductivities and storage parameters may change over time, as discussed <u>here</u>.

Initial Heads

In order to start solving the flow simulation, flow engines require an initial "guess" for the head values in the model. A good initial guess for the starting heads of the simulation can reduce the required run time significantly, while a poor initial guess can increase run times or lead to stability and/or convergence issues. The Initial Head values are also used to calculate drawdown values, as measured by the difference between the starting head and the calculated head.

Vadose Zone

The vadose zone object is only available when an unsaturated flow model (MODFLOW-2005 with the unsaturated zone flow (UZF) package or MODFLOW-SURFACT) is selected in the <u>Modeling Objectives</u> workflow step.

The vadose zone, or unsaturated zone, extends from the land surface to the water table. The vadose zone typically has a lower hydraulic conductivity because some of the pore space is filled with air, and the soil moisture in the vadose zone only travels through the wetted cross-section of the pore space. The relative proportion of air to water in the pores can vary, and consequently the hydraulic properties of the porous media can also vary.

In general, soil moisture in the vadose zone is under tension, and it travels through the vadose zone due to total soil-moisture potential (the sum of the elevation potential, and the pressure head). The pressure head is a function of the volumetric water content of the soil, and depends upon whether the soil has previously undergone wetting or drying. The relationship between pressure head and volumetric water content for a particular soil is known as a soil-water characteristic curve. Using the experimental soil-water characteristic curve and the soil hydrologic parameters, the movement of water in the vadose zone can be

determined using the BCF4 package in MODFLOW-SURFACT or the UZF package in MODFLOW 2005. A sample index of soil properties is given below:

Soil Type	Sand [%]	Clay [%]	Bulk Densi ty [g/cm ³]	Field Capa city [cm ³/cm³] *	Wiltin g Point [cm ³/cm³] **	Poros ity Fracti on [-]	Satur ated Hydra ulic Cond uctivi ty [cm/s]	Slope of Reten tion Curve [log space] ***	Van Genu chten Alpha para meter [cm ⁻¹]
sand (s)	94.83	2.27	1.49	0.08	0.03	0.43	0.0107	4.1	0.145
loamy sand (ls)	85.23	6.53	1.52	0.15	0.06	0.42	0.003	3.99	0.124
sandy loam (sl)	69.28	12.48	1.57	0.21	0.09	0.4	0.0015	4.84	0.075
silt loam (sil)	19.28	17.11	1.42	0.32	0.12	0.46	0.0011	3.79	0.02
silt (si)	4.5	8.3	1.28	0.28	0.08	0.52	0.0023	3.05	0.016
loam (I)	41	20.69	1.49	0.29	0.14	0.43	0.0005	5.3	0.036
sandy clay loam (scl)	60.97	26.33	1.6	0.27	0.17	0.39	0.0007	8.66	0.059
silty clay loam (sicl)	9.04	33.05	1.38	0.36	0.21	0.48	0.0015	7.48	0.01
clay loam (cl)	30.08	33.46	1.43	0.34	0.21	0.46	0.0005	8.02	0.019
sandy clay (sc)	50.32	39.3	1.57	0.31	0.23	0.41	0.0003	13	0.027
silty clay (sic)	8.18	44.58	1.35	0.37	0.25	0.49	0.0008	9.76	0.005
clay (c)	24.71	52.46	1.39	0.36	0.27	0.47	0.0009	12.28	

Table: Sample Index of Soil Hydraulic Properties by Soil Texture

Source: "Average hydraulic conductivity properties of ARS soil texture classes", draft dated February, 2000 by J. Schaake. This expanded the work of others and included a total of 2128 soil samples.

* Field capacity is the fractional water content at 1/3 bar tension.

** Wilting point is the fractional water content at 15 bar tension;

*** Used in Campbell's equation. ref: Coby et al. (1984)

**** Average values of the van Genuchten soil parameters obtained by experimental means (Carsel and Parrish, <u>1988</u>) and also reported on page 180 in Contaminant Hydrogeology book by C. W. Fetter (<u>1999</u>). You may also want to consider the ROSETTA code for estimating the unsaturated soil hydraulic properties which can be downloaded from the US Salinity Laboratory website: <u>https://data.nal.usda.gov/dataset/rosetta</u>.

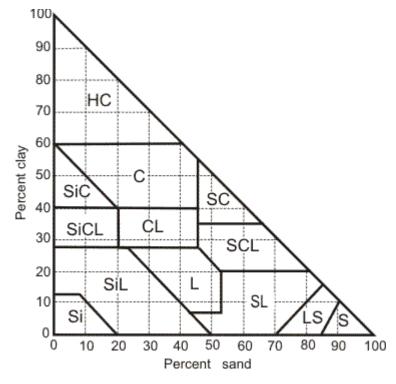


Figure: Soil texture classes triangle.

Source: Agriculture and Food Canada, 2017 (http://sis.agr.gc.ca/cansis/taxa/cssc3/chpt17.html)

Unsaturated Flow - UZF Package

In order to solve the variably saturated flow problem using the UZF package, it is necessary to specify the relationship of both the relative permeability (K_{rw}) and total pressure head (ψ) as functions of the water phase saturation (θ). Flow through and storage in the unsaturated zone is estimated in the UZF package using a kinematic wave approximation of Richard's equation using the method of characteristics. The approach includes the assumptions that flow in the unsaturated zone is driven by gravity, that negative potential gradients are ignored, and that flow is vertical through a homogenous column of soil. The Brooks-Corey function (Brooks-Corey, <u>1966</u>) is used to estimate the relationship between relative hydraulic conductivity and water saturation:

$$K_{rw} = S_e^{\ \varepsilon} = \left(\frac{\theta - \theta_r}{1 - \theta_r}\right)^{\varepsilon}$$

where:

 K_{rw} is the relative hydraulic conductivity [L/T]

e is the Brooks-Corey exponent [-]

 S_e is the effective water saturation [-]

 θ is the current water saturation, which is a function of pressure head [-]

 θ_r is the residual water saturation [-]

The parameters are entered as follows:

- EPS (Brooks-Corey exponent ε) controls the air-entry pressure the smaller the a value, the larger the capillary fringe above the water table. Gravels and sands have a large α while clayey soils have a small a.
- **THTi** (initial water saturation θ_i) initial water content in the vadose zone.
- THTs (residual water saturation θ_r) depends upon several factors of the soil including packing. Residual saturation values are generally low for sands and gravels and high for clayey soils. Residual saturation typically ranges from 0.01 to 0.4.

In addition to the property values described above, the UZF also includes transient boundary condition parameters for potential infiltration rates, potential evapotranspiration rates, extinction water depth and water content, as described in the boundary conditions theory section.

Unsaturated Flow - MODFLOW-SURFACT

The BCF4 package in MODFLOW SURFACT can solve for variably saturated flow in the vadose zone in three dimensions using the Brooks-Corey equation described above or using the Van Genuchten (1980) equation for relative permeability:

$$K_{rw} = S_e^{1/2} \left[1 - \left(1 - S_e^{1/\gamma} \right)^{\gamma} \right]^2$$

where:

 γ is an empirical parameter [dimensionless]

The relationship of the pressure head (ψ) [L] to relative saturation is described by van Genuchten (1980) using the following equation:

$$S_e = \left[\frac{\theta - \theta_r}{1 - \theta_r}\right] = \left[\begin{bmatrix} 1 + (\alpha h_c)^{\beta} \end{bmatrix}^{-\gamma} \dots for \dots \psi < 0\\ 1 \dots \dots for \dots \psi \ge 0 \end{bmatrix}$$

where:

 α is an empirical parameter [1/L]

 β is an empirical parameter [-] and is related to empirical parameter γ as follows: $\gamma = 1 - 1/\beta$

 h_c is the capillary pressure [L] and is related to pressure head (ψ) and elevation (z) by $h_c = \psi - z$

Depending on the saturation model selected, the primary inputs for simulating groundwater flow in the vadose zone using MODFLOW-SURFACT are the van Genuchten parameters (a, β , and θ_r) and the Brooks-Corey parameter (*e*). The Brooks-Corey and van Genuchten

empirical parameters can be measured in the laboratory for a given soil by plotting a soilwater characteristic curve.

The parameters are entered as follows:

- VANAL (van Genuchten α parameter) controls the air-entry pressure the smaller the α value, the larger the capillary fringe above the water table. Gravels and sands have a large α while clayey soils have a small a.
- VANBT (van Genuchten β parameter) controls how rapidly the saturation drops from unity to residual, and is an indicator of the grain size distribution. For larger values of β, the saturation drops rapidly with head (uniform grain size distribution), while for smaller values of β, the drop is more gradual (grain-size, and therefore pore size is more varied). β is greater than unity, but typically can be from 1.3 to 6, depending upon the soil.
- VANSR (residual water saturation θ_n) depends upon several factors of the soil including packing. Residual saturation values are generally low for sands and gravels and high for clayey soils. Residual saturation typically ranges from 0.01 to 0.4.
- Brook (Brooks-Corey ε) is the Brooks-Corey empirical exponent. It must be greater than zero (default value is 0.5).

Unsaturated Flow - Vapor Flow MODFLOW-SURFACT

The BCF4 package in SURFACT can also be used to simulate vapor flow through the vadose zone. Pressure head in the air phase (P_a) and total head in the air phase (h_{ap}) are related as follows:

$$h_a p = \frac{P_a}{\rho_w g} = h_{a\phi} - \frac{\rho_a}{\rho_w} z$$

where:

 ρ_w is density of water [L³/T]

 ρ_a is the density of air [L³/T]

g is the gravitational acceleration constant [L/T²]

 h_{ab} is the total head in the air phase [L]

z is the elevation [L]

Soil vapor flow options for MODFLOW-SURFACT simulations are set using the advanced settings for the BCF4 package in the <u>Translation Settings</u> workflow step. These are initially based on the project defaults for physical constants in the Model Defaults tab (found under *File / Project Defaults / Model Defaults*) and include the following:

RHOWP (ρ_w) is density of water [L³/T]

PHOAP (ρ_a) is the density of air [L³/T]

VISW (μ_w) is the viscosity of water [M/LT] **VISG** (μ_a) is the viscosity of air [M/LT] **COMPWAT** (β_w) compressibility of water [LT²/M] **COMPAIR** (β_a) compressibility of air [LT²/M] **ATMGP** (P_{atm}) is the standard atmospheric pressure [M/LT²] **GRAV** (g) is the gravitational acceleration constant [L/T²]

Transport Properties

If transport has been enabled at the <u>Define Modeling Objectives</u> step, then you may chose modeling objectives for the transport simulations, which include selections for the retardation and reaction models. If a transport engine has been selected then one or more of the following properties must be defined.

Initial Concentration

In many cases, the historical conditions of the site are unknown, and the contaminant source has been removed or remediated. In such cases, the groundwater contamination is still present and the mass transport simulation must be run forward in time, starting from the existing conditions, to predict the potential downstream impacts. The Initial Concentration properties define the existing conditions of each chemical species at the start of the simulation period.

Initial Concentrations must be defined for each chemical species that you have defined in the Define Modeling Objectives; the default value is 0. Furthermore, if you have selected a dual or multi-domain model, then initial concentrations must be defined for each species in each immobile domain.

Retardation Models

Visual MODFLOW Flex supports a variety of retardation and sorption models for solute transport.

Retardation

Retardation is a transport process that slows solute migration.

$$V_{R(i)} = \frac{V}{R_i}$$

where:

 $V_{R(i)}$ is the retarded flow velocity of species *i* [L/T]

V is the average linear groundwater flow velocity [L/T]

 R_i is the retardation coefficient of species *i*[-]

There are four sorption models for calculating the retardation, as described below:

Linear Sorption:

In linear sorption, the sorbed concentration is assumed to be directly proportional to the dissolved concentration in the adjacent pore space:

$$\overline{C_i} = K_{d(i)} \cdot C_i$$

where:

 $\overline{C_i}$ is the sorbed concentration of species *i* [M/M] \rightarrow [-]

 C_i is the dissolved concentration of species *i* [M/L³]

 $K_{d(i)}$ is the distribution coefficient of species *i* [L³/M]

The retardation coefficient for linear sorption is calculated as:

$$R_i = 1 + \left(\frac{\rho_b}{\phi} \times K_{d(i)}\right)$$

where:

 R_i is the retardation coefficient of species *i*[-]

 ρ_b is the dry bulk density of the soil [M/L³]

 ϕ_e is the effective porosity of the soil [L³/L³] \rightarrow [-]

 $K_{d(i)}$ is the distribution coefficient of species *i* [L³/M]

When the Linear Sorption model is included in a Transport Simulation, Visual MODFLOW Flex requires the following parameters:

Species Parameters

• Kd is a species parameter for the distribution coefficient [1/(M/L³)]

Model Parameters

• RHOB is the bulk density of the porous media [M/L³].

If a dual domain or multi domain model objective is specified (see below), then one or more of the following parameters may also be added:

Species Parameters

• KdIm (or KdIm1) is the species parameter for distribution in the (first) immobile domain [1/(M/L³)]

- KdIm2 is the species parameter for distribution in the (second) immobile domain [1/ (M/L³)]
- KdIm3 is the species parameter for distribution in the (third) immobile domain [1/ (M/L³)]

Model Parameters

- Rholm (or RHOBim1) is the bulk density of the porous media in the first immobile domain [M/L³]
- **RHOBim2** is the bulk density of the porous media in the second immobile domain [M/L³]
- RHOBim3 is the bulk density of the porous media in the third immobile domain [M/L3]

Freundlich Isotherm

The Freundlich Isotherm simulates sorption using an exponential function:

$$\overline{C_i} = K_{f(i)} \cdot C_i^{a_i}$$

where:

 $\overline{C_i}$ is the sorbed concentration of species *i* [M/M] \rightarrow [-]

 C_i is the dissolved concentration of species *i* [M/L³]

 $K_{f(i)}$ is the empirical Freundlich constant of species *i* [(L³/M)^a]

 a_i is the empirical Freundlich exponent of species *i*[-]

The retardation coefficient for the Freundlich isotherm is calculated as:

$$R_i = 1 + \left(\frac{\rho_b}{\phi_e} \times a_i K_f C^{a_i - 1}\right)$$

where:

 R_i is the retardation coefficient of species i [-]

 ρ_{b} is the dry bulk density of the soil [M/L³]

 ϕ_e is the effective porosity of the soil [L³/L³] \rightarrow [-]

 $K_{f(i)}$ is the empirical Freundlich constant of species $i [(L^3/M)^a]$

 a_i is the empirical Freundlich exponent of species *i*[-]

When the Freundlich Isotherm model is included in a Transport Simulation, Visual MODFLOW Flex requires the following parameters:

Species Parameters (one value per cell per species)

- Kf is the Freundlich constant [1/(M/L³)^a]
- **a** Freundlich exponent [-]

Note: MODFLOW-SURFACT also includes support for specifiying a different set of Freundlich isotherm parameters for the immobile domain:

- Kflm is the Freundlich constant in the immobile domain [1/(M/L³)^a]
- aim is the Freundlich exponent in the immobile domain [-]

Model Parameters (one value per cell)

• RHOB is the bulk density of the porous media [M/L³]

Langmuir Isotherm

The Langmuir Isotherm simulates sorption as a non-linear empirical function:

$$\overline{C_i} = \frac{\overline{S}K_{l(i)}C_i}{1 + K_{l(i)}C_i}$$

where:

 $\overline{C_i}$ is the sorbed concentration of species $i [M/M] \rightarrow [-]$

 C_i is the dissolved concentration of species *i* [M/L³]

 \overline{S} is the total concentration of sorption sites available for species $i [M/M] \rightarrow [-]$

 $K_{l(i)}$ is the empirical Langmuir constant of species $i [1/(M/L^3)]$

The retardation coefficient for Langmuir isotherm is calculated as:

$$R_{i} = 1 + \left(\frac{\rho_{b}}{\phi_{e}} \times \frac{\overline{S}K_{l(i)}}{\left(1 + K_{l(i)}C_{i}\right)^{2}}\right)$$

where:

 R_i is the retardation coefficient of species i [-]

 ρ_b is the dry bulk density of the soil [M/L³]

 ϕ_e is the effective porosity of the soil [L³/L³] \rightarrow [-]

 \overline{S} is the total concentration of sorption sites available for species *i* [M/M] \rightarrow [-]

 $K_{l(i)}$ is the empirical Langmuir constant of species *i* [1/(M/L³)]

When the Freundlich Isotherm model is included in a Transport Simulation, Visual MODFLOW Flex requires the following parameters:

Species Parameters (one value per cell per species)

- KI is the empirical Langmuir constant [1/(M/L³)]
- S is the total concentration of sorption sites available [M/M] \rightarrow [-]

Model Parameters (one value per cell)

• RHOB is the bulk density of the porous media [M/L³]

First Order Kinetic Sorption

The sorption models described above all assume that solute mass transfer between the dissolved and sorbed phases is instantaneous and in equilibrium. In some cases, this assumption may not be valid and sorption may be represented as a first-order reversible kinetic reaction:

$$\frac{\delta\overline{C_i}}{\delta t} = \left(\frac{\beta_i}{\rho_b}\right) \left(C_i - \frac{\overline{C_i}}{K_{d(i)}}\right)$$

where:

 $\overline{C_i}$ is the sorbed concentration of species *i* [M/M] \rightarrow [-]

 C_i is the dissolved concentration of species *i* [M/L³]

 ρ_b is the dry bulk density of the soil [M/L³]

 β_i is the first-order kinetic mass transfer rate between the dissolved and sorbed phase for species *i* [1/T]

 $K_{d(i)}$ is the distribution coefficient of species *i* [L³/M]

The retardation rate cannot be solved directly in the case of first order kinetic sorption. Instead, the above equation must incorporated into the governing transport equation and the sorbed/dissolved phase concentrations must be solved simultaneously. As the value of the mass transfer rate (β_i) increases, the system will tend towards the linear sorption model and as values of β_i decrease, the system will tend towards negligible sorption.

Dual Domain and Multi Domain Mass Transfer

Heterogeneous groundwater systems may be conceptualized as a dual or multi domain system. In such cases, the conceptualized system consists of a primary mobile domain where advection is a dominant transport mechanism and one or more adjacent immobile domains where advection is negligible relative to transport in the mobile domain. Solute mass transfer between the mobile and immobile domain(s) can be approximated as a first-order concentration gradient-driven diffusion-based mass balance for the *j*th immobile domain is calculated as:

$$\phi_{im(j)} \frac{\delta C_{im(ij)}}{\delta t} = \zeta_j \Big(C_i - C_{im(ij)} \Big)$$

where:

 C_i is the dissolved concentration of species *i* in the mobile domain [M/L³]

 $C_{im(ij)}$ is the dissolved concentration of species *i* in the *j*th immobile domain [M/L³]

t is time [T]

 ζ_j is the first-order mass transfer rate between the mobile domain and the *j*th immobile domain for species *i* [1/T]

 $\phi_{im(j)}$ is the porosity of the *j*th immobile domain. For dual-domain systems θ_{im} is typically assumed to be the difference between total porosity (ϕ_T) and effective porosity (ϕ_e) [L³/L³] \rightarrow [-]

Mass transfer between immobile domains is assumed to be negligible and is not included in the formulation.

If linear sorption is included in the modeling objectives, the mass balance for the *j*th immobile domain is calculated as:

$$\left(\phi_{im(j)} + f_{im(j)}\rho_{b[im(j)]}K_{d[im(ij)]}\right)\frac{\delta C_{im(ij)}}{\delta t} = \zeta_j \left(C_i - C_{im(ij)}\right)$$

where:

 $f_{im(j)}$ is the fraction of the *j*th immobile domain [-]

 $\rho_{b[im(j)]}$ is the bulk density of the *j*th immobile domain; in most cases $\rho_{b[im(j)]}$ is assumed to be the same as the bulk density of the mobile fraction [M/L³]

 $K_{d[im(ij)]}$ is the linear distribution coefficient for species *i* in the *j*th immobile domain $[1/(M/L^3)]$

The implementations in MT3D-MS and MODFLO-6 assume that $f_{im} = \phi_{im}/\phi_e$ and as such, it is not parameterized. The MODFLOW-SURFACT formulation of the transport equation defines the fraction of the immobile domain f_{im} as the difference between the total unit volume of aquifer (1) and the fraction of the mobile domain f_m , that is $f_{im} = (1 - f_m)$ and f_m is included as a parameter (PHIF).

Similar equations to the one above can be derived for non-linear sorption isotherms, as described in the MODFLOW-SURFACT Manual (HydroGeoLogic Inc., <u>1996</u>), which also supports the Freundlich Isotherm as part of a dual domain formulation. However, for the other transport engines supported by Visual MODFLOW Flex that implement a dual domain formulation (e.g. MT3D-MS and MODFLOW-6) are more restrictive; if a dual or multi-domain approach is included in the modeling objectives:

- MT3D-MS supports models with linear sorption in the mobile domain only
- MODFLOW-6 supports models with Freundlich isotherm or Langmuir isotherm sorption if and only if sorption is not simulated in the immobile domain(s). However, linear sorption may be simulated in some, all, or none of the mobile and immobile domain(s).

It should also be noted that MT3D-MS and MODFLOW-SURFACT only support dual domain formulations (i.e. a mobile domain and a single immobile domain. MODFLOW-6 allows support for an unspecified number of immobile domains; however, the Visual MODFLOW

Flex interface limits the number of immobile domains to three (as supported by the modeling objective entitled "Quadruple Domain with Complex Sorption").

Decay reactions may also be included in the above formulation. For more details, please refer to the documentation for the relevant transport engine:

- MT3D-MS: Zheng, C., and Wang, P., 1999. MT3DMS, A Modular Three-Dimensional Multi-species Transport Model for Simulation of Advection, Dispersion, and Chemical Reactions of Contaminants in Groundwater Systems: Documentation and User's Guide. U. S. Army Corps of Engineers, U. S. Army Engineer Research and Development Center, Vicksburg, Mississippi, SERDP-99-1.
- MODFLOW-6: Langevin, C.D., Provost, A.M., Panday, S., and Hughes, J.D., 2022. Documentation for the MODFLOW 6 Groundwater Transport Model: U.S. Geological Survey Techniques and Methods, book 6, chap. A61, 56 p., https://doi.org/10.3133/tm6A61.
- **MODFLOW-SURFACT**: HydroGeoLogic, Inc., 1996. *MODFLOW-SURFACT ver. 2.2* User's manual. A three dimensional fully integrated finite difference code for simulating Fluid flow and Transport of contaminant in saturated-unsaturated porous media. Herndon, VA 20170, USA.

When a dual domain or multi domain retardation model is included in a Transport Simulation, Visual MODFLOW Flex may require one or more of the parameters following may be required:

Species Parameters

- Kd is the species parameter for the distribution coefficient in the mobile domain [1/ (M/L³)]
- KI is the species parameter for the Langmuir is constant in the mobile domain [1/ (M/L³)]
- **S** is the species parameter for the total concentration of sorption sites available in the mobile domain [-]
- Kf is the species parameter for the Freundlich isotherm constant in the mobile domain [1/(M/L³)^a]
- a is the species parameter for the Freundlich exponent in the mobile domain [-]
- K_mass (or K_mass1) is the mass transfer rate between the mobile domain and the (first) immobile domain [1/T]
- K_mass2 is the mass transfer rate between the mobile domain and the (second) immobile domain [1/T]
- K_mass3) is the mass transfer rate between the mobile domain and the (third) immobile domain [1/T]
- KdIm (or KdIm1) is the species parameter for the distribution coefficient in the (first) immobile domain [1/(M/L³)]
- KdIm2 is the species parameter for the distribution coefficient in the (second) immobile domain [1/(M/L³)]
- KdIm3 is the species parameter for the distribution coefficient in the (third) immobile domain [1/(M/L³)]

Model Parameters

- RhobIm (or RHOBim1) is the bulk density of the porous media in the first immobile domain [M/L³]
- **RHOBim2** is the bulk density of the porous media in the second immobile domain [M/L³]
- RHOBim3 is the bulk density of the porous media in the third immobile domain [M/L3]
- PhiF is the volumetric fraction of the mobile domain relative to the model domain [-]
- Philm (or Philm1) is the porosity of the (first) immobile domain [-]
- Philm2 is the porosity of the second immobile domain [-]
- Philm3 is the porosity of the third immobile domain [-]

• Notes:

- Additional species parameters may be required if a non-trivial reaction model is selected (see below).
- Some species and model parameters have different names depending on which soprtion model is specified (e.g. K_mass vs K_mass1). These have the same physical meaning; this first name listed is for the specific dual-domain sorption models, whereas the second name is for the dual-, triple-, and quadruple-domain with complex sorption options supported by MODFLOW-6, which necessitate a numeric suffix to identify/differentiate the indices of the immobile domain(s).

Reaction Models

Visual MODFLOW Flex supports a variety of reaction for solute transport:

First-Order Irreversible Decay

In first order irreversible decay, the rate of change of solute concentration is proportional to the concentration at a given time. The mass balance term for first order decay as a function of time, (assuming no other processes), is given by:

$$\frac{\delta\left(\phi_{e}C_{t(i)}\right)}{\delta t} = -\lambda_{1(i)}\phi_{e}C_{t(i)}$$

where:

 $C_{t(i)}$ is the concentration of species *i* at time *t* [M/L3]

 $C_{0(i)}$ is the initial concentration of species *i* [M/L3]

 ϕ_e is the effective porosity of the soil [L³/L³] \rightarrow [-]

 $\lambda_{1(i)}$ is the first order decay rate of species *i* [1/T]

t is elapsed time [T]

Assuming the effective porosity does not change over time, ϕ_e can be dropped from both sides of the equation and the general solution for the concentration as a function of time is given by:

$$C_{t(i)} = C_{0(i)} e^{-\lambda_{1(i)}t}$$

First-order decay rate coefficients can be derived from half-life values, which are more commonly available. The half-life is the time for the constituent concentration to reach half of its initial concentration (i.e. $C_{t(i)} = 0.5 \times C_{0(i)}$). The first order decay rate is related to the half-life as follows:

$$\lambda_{1(i)} = \frac{\ln(2)}{t_{1/2(i)}}$$

where:

 $\lambda_{1(i)}$ is the first order decay rate of species *i* [1/T]

 $t_{1/2}(i)$ is the half-life of species *i* [T]

The first order decay may be applied to the constituent in supported phases (dissolved or sorbed) and/or domains (mobile or immobile), as supported by the various transport engines. Please refer to the descriptions of <u>Modeling Objectives</u> and <u>Species Parameters</u> for details.

When first order decay (or complex Model Reactions) is included in a Transport Simulation, Visual MODFLOW Flex may require one or more of the parameters following may be required:

- **K_mobile** is the first-order decay rate coefficient for dissolved constituents in both the mobile (and immobile domain, if applicable) [1/T]
- K_sorbed is the first-order decay rate coefficient for sorbed constituents in both the mobile (and immobile domain, if applicable) [1/T]
- K1 is the first-order decay rate coefficient for dissolved constituents in the mobile domain [1/T]
- **K1_sorbed** is the first-order decay rate coefficient for sorbed constituents in the mobile domain [1/T]
- K1_im1 is the first-order decay rate coefficient for dissolved consitituents in the first immobile domain [1/T]
- K1_im1_sorbed is the first-order decay rate coefficient for sorbed consitituents in the first immobile domain [1/T]
- K1_im2 is the first-order decay rate coefficient for dissolved consitituents in the second immobile domain [1/T]

- K1_im2_sorbed is the first-order decay rate coefficient for sorbed consitituents in the second immobile domain [1/T]
- **K1_im3** is the first-order decay rate coefficient for dissolved consitituents in the third immobile domain [1/T]
- K1_im3_sorbed is the first-order decay rate coefficient for sorbed consitituents in the third immobile domain [1/T]

Zeroth-Order Irreversible Decay

In zeroth order irreversible decay, the rate of change of solute concentration is constant. Zeroth order decay is most commonly used in situations where bio-geochemical decay (or production) does not depend on solute concentration or when simulating groundwater age, where the groundwater age where the is mathematically analogous to a solute (Goode, 1996). The mass balance term for zeroth order decay as a function of time, (assuming no other processes), is given by:

$$\frac{\delta\left(\phi_{e}C_{t(i)}\right)}{\delta t} = \pm \lambda_{0(i)}\phi_{e}$$

where:

 $C_{t(i)}$ is the concentration of species *i* at time *t* [M/L3]

 ϕ_e is the effective porosity of the soil [L³/L³] \rightarrow [-]

 $\lambda_{0(i)}$ is the zeroth order decay rate of species *i* [1/T]

t is elapsed time [T]

A negative value indicates a loss in mass concentration, which is commonly used models of bio-geochemical decay. A positive value of the zeroth order decay rate indicates a gain in mass concentration, which may be used for simulating a daughter product in some bio-geochemical reactions or for simulating groundwater age as the groundwater ages at a constant rate, (unless the some of the groundwater is accelerated to relativistic speeds, which is generally improbable and also apt to cause significant problems). Assuming the effective porosity does not change over time, ϕ_e can be dropped from both sides of the equation and the general solution for the concentration as a function of time is given by:

$$C_{t(i)} = C_{0(i)} + -\lambda_{0(i)}t$$

When zeroth order decay (or complex Model Reactions) is included in a Transport Simulation, Visual MODFLOW Flex may require one or more of the parameters following may be required:

- **K_mobile** is the zeroth-order decay rate coefficient for dissolved constituents in both the mobile (and immobile domain, if applicable) [1/T]
- **K_sorbed** is the zeroth-order decay rate coefficient for sorbed constituents in both the mobile (and immobile domain, if applicable) [1/T]

- K0 is the zeroth-order decay rate coefficient for dissolved constituents in the mobile domain [1/T]
- **K0_sorbed** is the zeroth-order decay rate coefficient for sorbed constituents in the mobile domain [1/T]
- K0_im1 is the zeroth-order decay rate coefficient for dissolved consitiuents in the first immobile domain [1/T]
- K0_im1_sorbed is the zeroth-order decay rate coefficient for sorbed consitituents in the first immobile domain [1/T]
- K0_im2 is the zeroth-order decay rate coefficient for dissolved consitituents in the second immobile domain [1/T]
- K0_im2_sorbed is the zeroth-order decay rate coefficient for sorbed consitituents in the second immobile domain [1/T]
- K0_im3 is the zeroth-order decay rate coefficient for dissolved consitituents in the third immobile domain [1/T]
- K0_im3_sorbed is the zeroth-order decay rate coefficient for sorbed consitituents in the third immobile domain [M/L]

RT3D Reaction Modules

RTD3 is an advanced transport engine that includes support for coupled reactions for several well known reaction types:

- Instantaneous aerobic degradation of of BTEX;
- Six-Species, First-Order, Rate-Limited, BTEX Degradation using Sequential Electron Acceptors;
- Rate-Limited Sorption;
- Double-Monod Model;
- Sequential First-Order Decay; or
- Aerobic/Anaerobic PCE/TCE Dechlorination

A description of these reactions is beyond the scope of the Visual MODFLOW Flex documentation as RT3D; however, the reactions are well descbribed in the RT3D documentation by Clement (<u>1997</u> and <u>2003</u>).

Dispersion

Dispersion is a physical process that tends to 'disperse', or spread, the solute mass in the X, Y and Z directions along the advective path of the plume, and acts to reduce the solute concentration (but not overall mass). Dispersion combines two physical processes,

mechanical dispersion (D^{mech}) which is due to the tortuosity of the flowpaths of the groundwater as the macro-scale as the solute travels through the interconnected pores of the soil and by diffusion (D^*) which is caused by random Fickian motion that tends to spread solute mass away from areas of higher concentration. Dispersion is calculated using the equation:

$$D = D^{mech} + D^* = \alpha_L \times \frac{v_L^2}{|v|} + \alpha_H \times \frac{v_H^2}{|v|} + \alpha_V \times \frac{v_V^2}{|v|} + D^*$$

where:

D is the Dispersion Coefficient [L²/T]

 D^{mech} is the Mechanical Dispersion Coefficient [L²/T]

 D^* is the diffusion coefficient [L²/T]

 α_L is the longitudinal dispersivity [L]

 v_L is the longitudinal velocity of flow along the plume migration pathway [L/T]

 α_{H} is the horizontal dispersivity [L]

 v_{H} is the horizontal velocity of flow along the plume migration pathway [L/T]

 α_V is the vertical dispersivity [L]

 v_V is the vertical velocity of flow along the plume migration pathway [L/T]

|v| is the magnitude of the groundwater velocity [L/T]

MT3DMS, RT3D, SEAWAT, and SURFACT

MT3DMS, RT3D, SEAWAT, and SURFACT calculate the Dispersion Coefficient for the mass transport model using the following parameters:

- Longitudinal Dispersivity (α_L) for each transport grid cell
- Ratio of Horizontal to Longitudinal Dispersivity (α_H/α_L) for each layer
- Ratio of Vertical to Longitudinal Dispersivity (α_V / α_L) for each layer
- Molecular Diffusion Coefficient for each layer

Longitudinal Dispersion can be defined using the regular set of tools provided for most parameters (i.e. cell-by-cell, by layer/row/column, or using polylines/polygons/data objects). The Longitudinal Dispersion can also be defined on a layer-by-layer basis by right-clicking the Longitudinal Dispersion object in the model tree and selecting the Dispersion Parameters option.

Transport Transport Transport Diritial Conc Director Species Pa Dulk Densit Densitudie=	rameters V
Cone Budget Cone Budget Constant Hea Constant Heads Obse Concentratio Coutputs	Flex Viewer Delete Edit Property Zones Settings Export Dispersion Parameters 3D Viewer Expand to selection Expand all child nodes Collapse all

The following dialog will appear:

😻 Di	spersion Parameters			- 🗆 ×
	Layer	Horiz/Long Dispersivity	Verti/Long Dispersivity	Diffusion Coeff. (m^2 / day)
•	1	0.1	0.01	0
	2	0.1	0.01	0
			(OK Cancel

Longitudinal Dispersion can also be defined based on property zones by right-clicking the Longitudinal Dispersion object in the model tree and selecting the Edit Property Zones... option. The absolute values of the horizontal and vertical dispersion parameters will be adjusted according to the property zone values.

t Cells Script	Longitudinal Dispersion	n 🖾 Calculat	tion			
					Diania	V
Zone	Layer	T F	Row T	Column V	Dispersion	Ŷ
1		1	1	10		
		1	2	10 10		
		4	3	10		
		4	4	10		
		4	- -	10		
		1	7	10		
		1	8	10		
	i	i	9	10		
	1	i	10	10		
	1	1	11	10		
	1	1	12	10		
	1	1	13	10		
	1	1	14	10		
	1	1	15	10		
	1	1	16	10		
	1	1	17	10		

For SEAWAT models, you can also specify a diffusion coefficient for each species using the MDCOEFF variable at the define modeling objectives step. The values will only be used if the Multi-Diffusion option is set to true in the <u>Advanced Settings</u> for the DSP package in the Translation step.

MODFLOW-6

MODFLOW-6 includes a more complex conceptualization of the Mechanical Dispersion tensor (please see Langevin, et al, <u>2022</u>) and calculates the Dispersion Coefficient for the mass transport model using the following parameters on a cell-by-cell basis:

- **ALH** is the longitudinal dispersivity in the horizontal direction. If flow is strictly horizontal, then this is the longitudinal dispersivity that will be used. If flow is not strictly horizontal or strictly vertical, then the longitudinal dispersivity (α_L) is a function of both ALH and ALV.
- **ALV** is the longitudinal dispersivity in vertical direction. If flow is strictly vertical, then this is the longitudinal dispersivity value that will be used. If flow is not strictly horizontal or strictly vertical, then the longitudinal dispersivity (α_L) is a function of both ALH and ALV.
- ATH1 is the transverse dispersivity in the horizontal direction. This is the transverse dispersivity value for the second ellipsoid axis. If flow is strictly horizontal and directed in the X direction, then this value controls spreading in the Y direction. If mechanical dispersion is represented (by specifying any dispersivity values) then this array is required.
- ATH2 is the transverse dispersivity in the horizontal direction. This is the transverse dispersivity value for the third ellipsoid axis. If flow is strictly horizontal and directed in the X direction, then this value controls spreading in the Z direction. If this value is not

specified and mechanical dispersion is represented, then this array is set equal to ATH1.

• **ATV** is the transverse dispersivity when flow is in vertical direction. If flow is strictly vertical and directed in the Z direction, then this value controls spreading in the X and Y directions. If this value is not specified and mechanical dispersion is represented, then this array is set equal to ATH2.

10.1.4.1 Dispersion Theory

The hydrodynamic dispersion tensor for an anisotropic medium is generally expressed as:

$$D = D_{ij}^{mech} + D_{ij}^{mol} = \begin{pmatrix} D_{xx}^{mech} & D_{xy}^{mech} & D_{xz}^{mech} \\ D_{yx}^{mech} & D_{yy}^{mech} & D_{yz}^{mech} \\ D_{zx}^{mech} & D_{zy}^{mech} & D_{zz}^{mech} \end{pmatrix} + D^{mol}I^*$$

$$\begin{split} D_{xx}^{mech} &= \alpha_{LH} \left(\frac{v_x^2}{v} \right) + \alpha_{TH_1} \left(\frac{v_y^2}{v} \right) + \left[\alpha_{TH_2} \left(\frac{v_x^2}{v^2} \right) + \alpha_{TV} \left(1 - \frac{v_x^2}{v^2} \right) \right] \left(\frac{v_z^2}{v} \right) \\ D_{yy}^{mech} &= \alpha_{TH_1} \left(\frac{v_x^2}{v} \right) + \alpha_{LH} \left(\frac{v_y^2}{v} \right) + \left[\alpha_{TH_2} \left(\frac{v_y^2}{v^2} \right) + \alpha_{TV} \left(1 - \frac{v_y^2}{v^2} \right) \right] \left(\frac{v_z^2}{v} \right) \\ D_{zz}^{mech} &= \alpha_{T_2} \left(\frac{v_x^2}{v} \right) + \left[\alpha_{LH} \left(1 - \frac{v_z^2}{v} \right) + \alpha_{LV} \left(\frac{v_z^2}{v^2} \right) \right] \left(\frac{v_y^2}{v} \right) + \left[\alpha_{TH_2} \left(\frac{v_y^2}{v^2} \right) + \alpha_{TV} \left(1 - \frac{v_y^2}{v^2} \right) \right] \left(\frac{v_z^2}{v} \right) \\ \end{split}$$

USG TRANSPORT

(Anisotropic Dispersion Terms

$$\begin{aligned} \theta_w D_{xx} &= \alpha_{LH} \left(\frac{v_x^2}{v} \right) + \alpha_{TH_1} \left(\frac{v_y^2}{v} \right) + \alpha_{Txz} \left(\frac{v_z^2}{v} \right) + \theta_w D^* \\ \theta_w D_{yy} &= \alpha_{Txy} \left(\frac{v_x^2}{v} \right) + \alpha_{LH} \left(\frac{v_y^2}{v} \right) + \alpha_{Tyz} \left(\frac{v_z^2}{v} \right) + \theta_w D^* \\ \theta_w D_{zz} &= \alpha_{Txz} \left(\frac{v_x^2}{v} \right) + \alpha_{Tyz} \left(\frac{v_y^2}{v} \right) + \alpha_{LV} \left(\frac{v_z^2}{v} \right) + \theta_w D^* \end{aligned}$$

Cross-Dispersion Terms

$$\theta_w D_{xy} = \theta_w D_{yx} = \left(\alpha_{Lxy} - \alpha_{Txy}\right) \left(\frac{\nu_x \nu_y}{\nu}\right)$$

$$\theta_{w}D_{xz} = \theta_{w}D_{zx} = (\alpha_{Lxz} - \alpha_{Txz})\left(\frac{v_{x}v_{z}}{v}\right)$$
$$\theta_{w}D_{yz} = \theta_{w}D_{zy} = (\alpha_{Lyz} - \alpha_{Tyz})\left(\frac{v_{y}v_{z}}{v}\right)$$

For simple cases:

$$D^{mech} = \begin{pmatrix} D_{xx}^{mech} & 0 & 0 \\ 0 & D_{yy}^{mech} & 0 \\ 0 & 0 & D_{zz}^{mech} \end{pmatrix}$$

where:

Q_t is the flow in/out of the well	
	[L ³ /T]

 \boldsymbol{r} is the effective radius of the well

[L]

10.2 Define Numerical Model

The next step is to choose to Import Model (import Visual MODFLOW Classic project or MODFLOW files), or Create Grid (create an empty grid).

🐯 Visual MODFLOW Flex - [Airport]		×
File View Tools Workflow Wind	ow Help	
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	AIRPORT4 grid-Run X Numerical Model X	
Data	00	
Area Chemiser 1 A	 Brench Montegorgersen Bre	

Import Model

You can import a Visual MODFLOW Classic project or a USGS MODFLOW 2000/2005 data set.

When you click on the Import Model button, the following dialog will appear:

🐯 Import Model					×
🗧 -> -> -^ 🔂 -> Thi	$s PC \rightarrow OS(C) \rightarrow Users \rightarrow Public \rightarrow Public D$	ocuments > Visual MODFLOW Flex		~ 0	P Search Visual MODFLOW Flex
Organize - New folde					ii • 💷 👔
Cycick access This PC Dotytosts Dostrop Downoods Mokic Pictures Videss Videss So(0)	None ^	Date modified 12/15/2013 140 944 3/11/2022 11:06 AA4	Type S File folder File folder	ize	
File na	me				All supported files (*.NAM, *.VF ~ Open Cancel

To import your Visual MODFLOW Classic project, select the .VMF file and click Open to continue.

To import a MODFLOW data set, change the file type to "MODFLOW 2000 or MODFLOW 2005", then select the desired .NAM file,and click Open to continue. A description of the limitations on models that can be imported is available <u>here</u>.

Once the model is finished importing, click 🕑 (Next Step) to proceed.

Create Grid

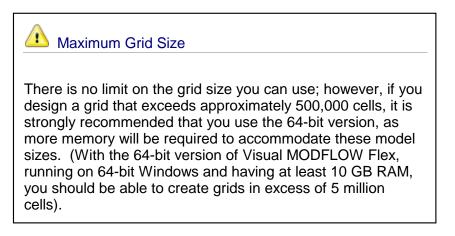
If you select the Create Grid option, the following window will appear.

umerical Model 🗙			
Ð			
Define Modeling Objectives Define Numerical Model	Name		Grid Preview
Create Grid	NumericGrid1	Create Grid	
Import Model	Rotation		
View/Edit Grid Define Properties	0	Edit Grid	
Define Boundary Conditions	Grid Size		
Select the Next Step	Rows Cell Height Max Ratio Threshold	Define Child Grid	
Define Observation Wells Define Zone Budget Zones	20 50.000 1.50 🜩		
Define Particles	Columns Cell Width	Add Data Object 🛶	
Select Run Type	20 50.000		
PEST Run Single Run	Grid Extents		
Translate	X Min X Max		
Run Numerical Engines	0 1000		
View Results	Y Min Y Max		
View Charts			
	 Calculate extents from a polygon object 		
	⇒		
	Number of Layers		
	2 -		
		Elevation	
	Layer Name Use Surface Surfaces	100	
	Layer 2 - Top	50	
	Layer 2 - Bottom	0	

At this step, you can define the Horizontal Grid (grid size and the extents), and the Vertical Grid (number of layers and the layer elevations).

Define Horizontal Grid

Define the Grid size (number of Columns and Rows), Rotation, and the Grid Extents. If you prefer you can also define the Cell Height and Width.



The grid extents can be defined manually; enter the min and max values for the X and Y coordinates.

Alternatively, the extents can be calculated from a bounding polygon. Select the option "Calculate extents from a polygon object". You will need to import a polygon object (from .SHP or .DXF File), that contains just a single, closed polygon, and provide this is as an input. For details on importing polygon objects, see the section <u>Import Polygons</u>. Once the polygon is imported, it will appear in the Data tree in the top left.

Select/click on this polygon from the Data tree, then click on the blue arrow button under "Calculate extents from a polygon". The polygon should appear, and the X and Y extents will be calculated accordingly.

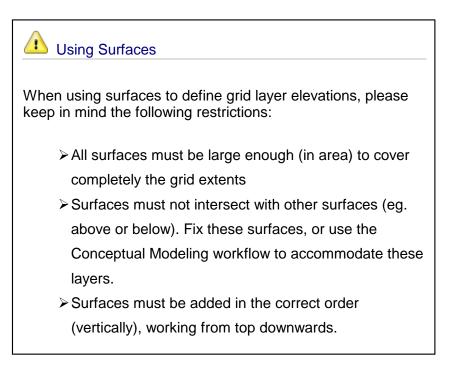
Please Note: Visual MODFLOW Flex will calculate a minimum bounding rectangle from an irregularly-shaped polygon, in order to calculate the X and Y min/max extents.

Define Vertical Grid

Specify the number of layers you want for the grid. In the table below, you can manually define a constant (flat) layer elevation for the top of each layer, and the bottom of the bottommost layer (by default, Visual MODFLOW Flex will calculate equally thick layers)

At this step, you can also defined varying layer elevations by using surfaces. This is intended for "simple" numerical models where "pancake-layer geology" is applicable. If your model has layers that pinchouts and/or discontinuities, it is advised that you follow the <u>Conceptual</u> <u>Model workflow</u>, as this will allow you to better accommodate more complex geology, using Horizon rules.

To define Surfaces for Grid layers, first you need to <u>import surfaces</u> (from Surfer .GRD, ESRI .ASC, etc.) or <u>create surfaces</u> from a set of points. Once the surfaces are available in the Data tree, select each surface for the appropriate layer elevation, being sure to work your way downwards (define top of layer 1 first, then work downwards).



Once you are finished defining the horizontal and vertical grid, click on the [Create Grid] button at the top (middle) of the window.

Once the grid is created, there are several options to customize the grid to your project needs.

The Edit Grid button will load a window where you can refine/coarsen the grid. For more details on this option, please see the <u>Edit Grid</u> section.

The Define Child Grid button will load a window where you can create child (local) grids for a MODFLOW-LGR run. For more details, please see the <u>Define Child Grid (for LGR)</u> section.

When you are finished with the grid edits, click on the S (Next Step) to proceed. This will generate the model tree structure (in the lower left corner of the window), with Inputs and Outputs.

10.3 View/Edit Grid

The View Edit/Grid Step allows you to review the grid once it has been created or imported.

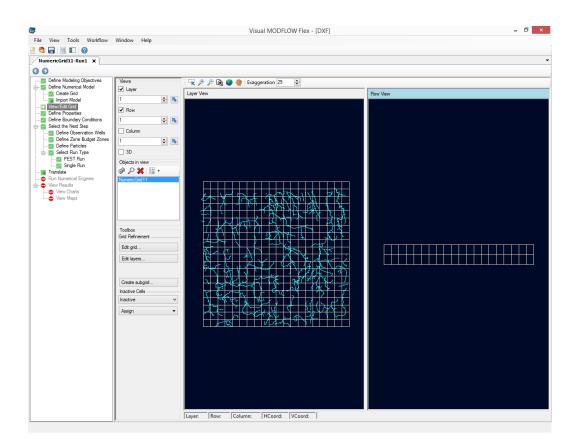
View/Edit Grid Step Availability

This step will <u>not</u> be shown if your model was converted from a conceptual model workflow to a numerical model workflow. If that is the case, you may edit the grid in the <u>Conceptual</u> <u>Modeling Workflow</u> using the same tools as presented below.

Visualizing the Grid

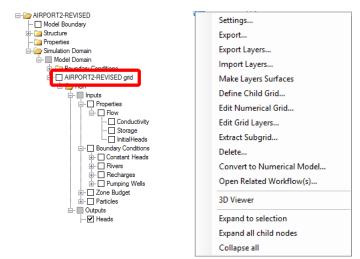
There are several options available for visualizing the grid:

- Under the Views section in the panel, you can select the various views you want to see in the Flex viewer: Visual MODFLOW Flex allows you to simultaneously show a layer, row, column and/or 3D subview.
- You can select which specific layer, row, and column is shown in the subviews by:
 o using the up/down arrows next to each,
 - o entering a specific row, column, or layer integer in the appropriate textbox, or
 - clicking on the button then clicking on any specific row, column, or layer in any of the 2D views
- The toolbar at the top of the views provides standard navigation tools allowing you to zoom, pan, and in the case of the 3D subview, rotate the view.



Context Menu

You can right-click on the numerical grid in the Model Explorer and select Settings. In addition, the Numerical Grid can be added to a stand-alone 3D view; to do this, right click and select 3D Viewer.



There are several other options available on the right click menu.

The numerical grid can be exported to shapefile; see Export for more details.

- **Export Layers**: allows you to export the layers of the grid to .txt or .csv file. These files can be edited and then imported back.
- Import Layers: allows you to import back the layers you exported (and edited).

You will also find the option to "Make Layers Surfaces" which will create a folder in the Data Explorer (named: grid name Layers Surfaces) where you will find that surfaces have been created for each layer starting with Top, followed by Bottom.001, Bottom.002 etc.

Grid Modification

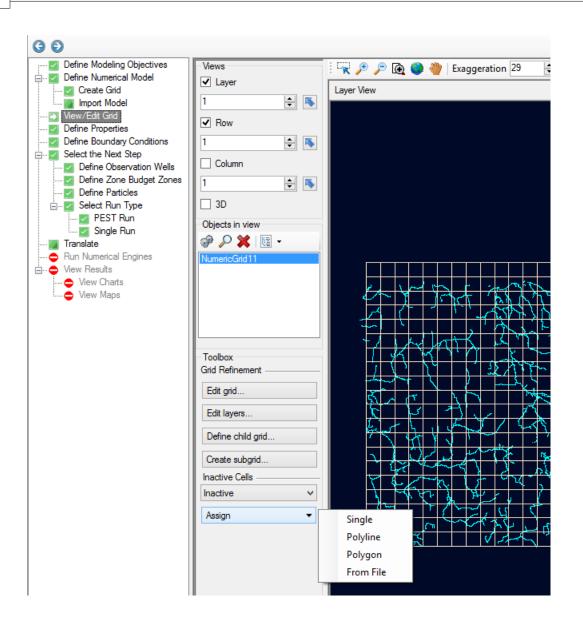
In the toolbox under the Grid Refinement section you have options to <u>Edit Numerical</u> <u>Grid...</u>... (horizonal) <u>Edit Grid Layers...</u> (vertical) as well as <u>Define Child Grid (for LGR)</u> and <u>Extract subgrid</u>.

Assign Active/Inactive Cells

At this step, you can digitize a polyline or polygon, and set the selected cells as inactive (or conversely, change inactive cells back to active cells)

- Select the desired flag from the combo box under "Inactive Cells" (make Active cells Inactive, or make Inactive cells Active)
- Select the Assign button.
- Choose the desired shape for drawing (Single, Polyline, Polygon)

640



- Use the left mouse button to start drawing in the grid view, and add highlight the desired cells; for single cell selection, a point will appear on top of the selected cell.
- Once you have finished digitizing, right click with the mouse and select "Define Attributes" (or click on the "Finish" button under the toolbox); the following window will appear.

Copy to Layer(s)	_	_		\times
Layer 1 Layer 2				
Layer 3				
	01/		0	
	<u>о</u> к		<u>C</u> ano	cel

- Choose which layers you wish to include in the cell assignments; by default, just the current layer is selected, however you can select other (or all) layers from this window
- Click OK
- The selected cells will be set as Inactive or Active, depending on the option you have selected. Inactive cells will be colored turquoise.

Assign from File

You can also assign cells as inactive (or active) based on an imported file. The required input format for the file is an ASCII text file that contains an U2DINT array of the model, as described by in the MODFLOW <u>documentation</u>. The array must have the correct number of values (i.e. number of rows times the number of columns). Examples of this type of array can be found in the [*model*].BAS.IBOUND[k] files in the translation folder of your model, where [*model*] is the base name of your model files and [k] is the layer number. Values in the array will affect change the (in)active state of each cell as follows:

- Cells corresponding to a positive integer in the array file will be set to the current selection of the Active/Inactive dropdown in the Toolbar.
- Cells corresponding to zero or negative values in the array file will not be changed

Once you have selected the file, you will be prompted to select which layer(s) the file will be applied to:

Copy to Layer(s)	_		\times
└ Layer 1 Layer 2 Layer 3			
	<u>о</u> к	<u>C</u> a	ncel

- Choose which layers you wish to include in the cell assignments; by default, just the current layer is selected, however you can select other (or all) layers from this window
- Click OK
- The selected cells will be set as Inactive or Active, as described above. Inactive cells will be colored turquoise.

When you are finished with viewing the grid, click ジ (Next Step) to proceed to the Define Properties step.

10.3.1 Edit Grid

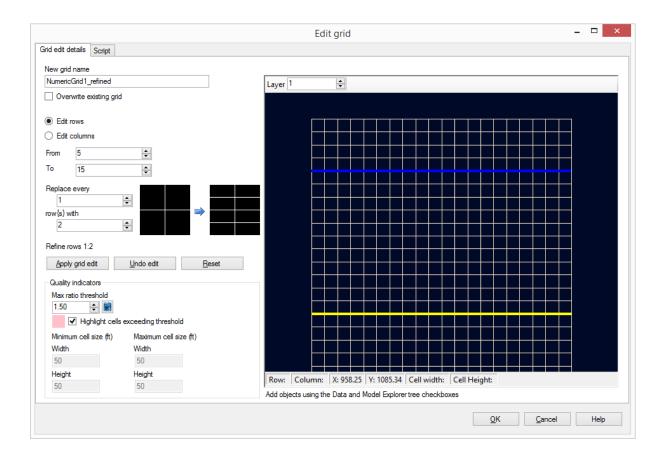
When a numerical grid is initially created (see "<u>Creating a Finite Difference Grid</u>" section), the horizontal grid spacing is uniform. However, in many situations it is advantageous to have non-uniform grid spacing to allow for finer grid discretization in the areas of interest, and larger grid spacing in areas which are less important, or where less data is available. Visual MODFLOW Flex allows you to refine or coarsen areas of a numerical grid by adding or removing grid lines within a specified row/column interval. This process is described in the following section.

Note	
You cannot edit a grid th grid (i.e. grid edits are n for LGR Models).	

To edit the grid (rows and columns) select the View/Edit Grid step of the Numerical Workflow and then select the Edit grid button. Alternatively, you can find this option from the Model Explorer tree, right-click on the Numerical Grid, and select Edit Numerical Grid from the pop-up menu.

The Edit grid dialog provides options for refining/coarsening a numerical grid.

When you edit the grid by default you are creating a new grid - and a default New grid name is generated (you can adjust this if you wish). If however, you prefer to simply overwrite your existing grid with the changes you make simply select the check box to do so.



Tip! You can add data objects (e.g., boundary conditions, wells, site maps) from the data explorer to the 2D Viewer preview to assist you in determining the areas in which horizontal refinement/coarsening should be applied. Select the desired data objects from the Data Explorer, and the data will be displayed in the 2D Viewer preview.

- Select the Edit Rows radio button to add/remove grid lines (rows) along the Y-direction of the numerical grid, or select the Edit columns radio button to add/remove grid lines (columns) along the X-direction of the numerical grid.
- Specify the row/column interval for which the refinement/coarsening should be applied, by specifying the From row/column and the To row/column. For example, if you would like to refine the grid area between row 20 and 30, you would enter 20 as the From row and 30 as the To row. In the preview the blue line represents the From row/column while the yellow line represents the To row/column.
- Next, specify the refinement/coarsening factor. In the example above we are going to Replace every 1 row with 2 so the grid will be refined. This means that we would subdivide each row within the specified interval into two equally spaced rows.

- Instead, if we changed the option to indicate we are going to Replace every 2 rows with 1 then the grid would be coarsened. This means we would reduce the number of rows within the specified interval by a factor of 2.
- When you select the Apply grid edit button the preview will be updated with your edits. You also have options to Undo your edit - this will undo your last change. You can keep selecting Undo edit to undo more changes. Reset will return the preview to the original rows and columns.
- Click the OK button to create the new refined/coarsened grid. You will find it in the Model Explorer.

When editing a grid all inputs from the original grid (property zones, boundary conditions, pumping wells, observation wells, zone budget zones, and particles) will be reassigned as appropriate to the new edited grid. If the original grid has multiple runs associated with it - the inputs are taken from the first run.

Quality Indicators

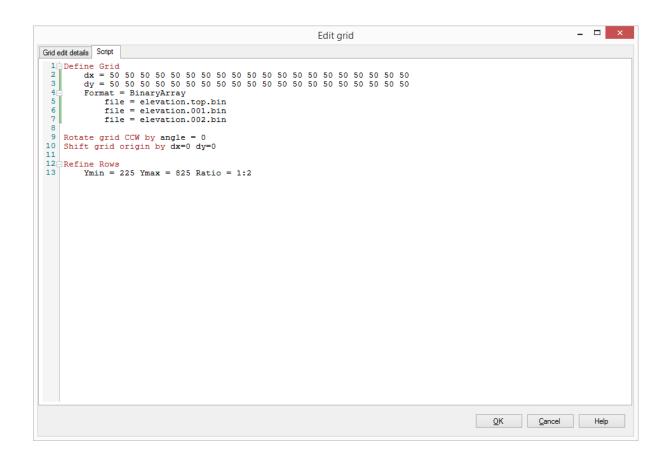
The quality indicators can help you find areas in your grid where you may wish to make adjustments. By default the Maximum ratio threshold is 1.5 however you can adjust this to your model requirements. If you do not wish to have the Quality indicators on simply uncheck the Highlight cells exceeding threshold option.

Also displayed in the Minimum and Maximum cell size.

Quality indicators	
Max ratio threshold	
1.55 🚖 🔃	
✓ Highlight cells	exceeding threshold
Minimum cell size (ft)	Maximum cell size (ft)
Width	Width
50	50
Height	Height
50	50

Script

If preferred, you can make your grid edits by using the Script option. On this tab you will find the script for any edits you make on the Grid edit details tab allowing you to learn the script language.



10.3.2 Edit Layers

To edit the grid (layers) select the View/Edit Grid step of the Numerical Workflow and then select the Edit layers button. Alternatively, you can find this option from the Model Explorer tree, right-click on the Numerical Grid, and select Edit Grid Layers from the pop-up menu.

The Edit layers dialog provides options for refining/coarsening/editing a numerical grid. When you edit the grid by default you are creating a new grid - and a default New grid name is generated (you can adjust this if you wish at the time the new grid is generated - once a grid is created, it cannot be renamed). If however, you prefer to simply overwrite your existing grid with the changes you make, simply select the check box to do so.

The dialog also provides you with a preview of the grid layers as viewed by a Row or a Column - you can select this from the Viewing drop down options above the preview window. You can then adjust which Row or Column you are viewing using the up and down arrows as well as the Exaggeration.

When you select the Apply edit button the preview will be updated with your edits. You also have options to Undo your edit - this will undo your last change. You can keep selecting Undo edit to undo more changes. Reset will return the preview to the original rows and columns.



You can add data objects (e.g., boundary conditions, wells, etc.) from the data explorer to the preview to assist you in determining the areas in which refinement/coarsening should be applied. Select the desired data objects from the Data Explorer, and the data will be displayed in the preview.

Edit Layers Dialog

The Edit Layers dialog provides several options for adjusting the layers of your model, including:

- Refine: subdivide one or more model layers by a (whole number) factor,
- Insert: subdivide a model layer by inserting a new surface into the model
- <u>Remove</u>: coarsen the model by removing a surface from the model
- <u>Replace</u>, adjust the elevation of a model layer by replacing the top (or bottom) elevations of a model layer
- Cells: adjust the elevations of individual cells
- <u>Script</u>: use a script to define the elevation of individual cells

These options are described in detail below.

Creating New Grids - Applying and Committing Edits to Grid Layers

To implement or preview any of the edits described below, first click the **Apply edit** button, you can where you can review and inspect the changes. You must click the Apply edit button for each individual change to the grid. Applied edit(s) to the grid layers will be saved into a new grid with the name entered under the **New grid name** option once you click the **OK** button. If you may choose to **overwrite the existing grid**, in which case the edited grid will replace the existing grid. If the current grid is associated with more than one model run (e.g. you have cloned one or more models associated with the grid or created updated run(s) using PEST, etc.) then you will be prompted to select which runs should be included with the updated/new grid layers.

ver edit details Script New grid name NumericalGrid_refined	Viewing Row 🗸 35 🌩 Exaggeration 20 卖 🔊 🔎 🌘 🍑 🦥
Overwrite existing grid Refine Insert Remove Replace Cells From layer 2 • To layer 5 • By a factor of 2	Layer: 1 Row: 1 Column: 1 X: -848.81 Z: 246.05
Apply edit Undo edit Reset	Add objects using the Data and Model Explorer tree checkboxes

Minimum Layer Thickness

Some layer editing options (i.e. insert and replace) include settings to ensure that edits to grid layer do not result in layers with thicknesses below a specified threshold (i.e. **the minimum layer thickness**) – this is an important consideration in grid design as models with overly thin model cells may result in numerical instabilities and convergence issues.

The default **minimum layer thickness** in Visual MODFLOW Flex is 0.1 measurement units (i.e. feet or meters).

Refine Insert Remove Replace Cells	Refine Insert Remove Replace Cells
Fraction of layer Thickness below layer ceiling Push down Thickness below layer ceiling	Top of layer Bottom of layer Push down
 Thickness above layer floor At elevation Layer 4 Fraction 0.01 	1 Use surface object New surface name Use elevation
Minimum layer thickness 0.10 🖨 m	1.00 m Minimum layer thickness 0.10

The **Push up** and **Push down** options are provided to determine how layers should be adjusted (if necessary) to so that resulting layers are not thinner than the specified threshold:

• When <u>neither</u> Push up nor Push down are selected, then the new surface (or applicable portions of the new surface) will be raised above existing surfaces below the insertion point and the new surface (or applicable portions of the new surface) will be lowered below existing surfaces above the insertion point such that the minimum layer

thickness criteria is obeyed. In this case, only (applicable portions of) the new surface will be adjusted to to enforce the minimum layer thickness criteria. If the elevation difference between the surfaces immediately above and below the new surface (or portions thereof) is less than twice the minimum thickness, the minimum layer thickness criteria will not be satisfied and you will be prompted with a warning message.

- When only <u>Push up</u> is selected, then applicable surfaces (or applicable portions of surface) above the new surface will be sequentially raised (pushed up) above this new surface such that the Minimum layer thickness criteria is obeyed. In this case, the layer below the new layer may push the new layer itself upwards and this push may propagate upwards through the model layers to enforce the minimum layer thickness criteria.
- When only <u>Push up</u> is selected, then applicable surfaces (or applicable portions of surface) above the new surface will be sequentially raised (pushed up) above this new surface such that the Minimum layer thickness criteria is obeyed. In this case, the layer above the new layer may push the new layer itself downwards and this push may propagate downwards through the model layers to enforce the minimum layer thickness criteria.
- When <u>both Push up and Push down</u> are selected, then the new surface will combine the individual behavior of when Push up or Push down are selected that is, the new surface will push (applicable portions of) surfaces above and below away from the new surface such that the minimum layer thickness criteria is obeyed. In this case, all layer adjustments would propagate outwards from the new layer and (applicable portions of) layers above and below the new layer may be adjusted to enforce the minimum layer thickness criteria.

Refine

You can select the **from layer** and **to layer** values and then provide a **Factor** to refine by. For example if you have 6 model layers and indicate the From 3 To 5 and a factor of 2 (as shown below) when you select the Apply edit button, you would end up with a total of 9 layers (as three of the original layers would remain unchanged and three of the layers would be split into 2).

er edit details Scr lew grid name NumericalGrid_refin	ed		Viewing Row 🔹 35 🐑 Exaggeration 20 😭 🔊 🔎 🚱 💙
Overwrite existin Refine Insert Insert I From layer 2 To layer 5 By a factor of 2	g grid Remove Replace Ce	ls	
Apply edit	Undo edit	Reset	Layer: 1 Row: 1 Column: 1 X: -848.81 Z: 246.05 Add objects using the Data and Model Explorer tree checkboxes

Insert

You can select to insert a new layer using the following options:

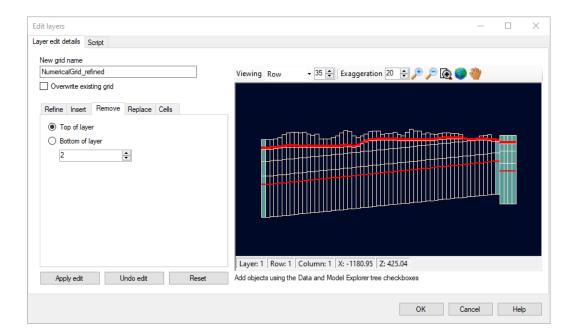
- Fraction of layer
- Thickness below layer ceiling
- Thickness above layer floor
- At elevation

When you select which option you want to use you will see in the preview that the selected layer is highlighted in green and when you hover your mouse over the preview the proposed new layer to be inserted will appear as a red line. You can also click on the grid to select where to place the inserted layer using the selected option (e.g. fraction, thickness, or constant elevation).

lew grid name NumericalGrid_refined] Overwrite existing grid	Viewing Row 🔹 35 🔃 Exaggeration 20 🏚 🍠 👰 🌺
Refine Insert Remove Replace Cells Fraction of layer Push up Thickness below layer ceiling Push down Thickness above layer floor At elevation Layer Image: Cells Image: Cells Remove above layer floor At elevation Layer Image: Cells Image: Cells	Layer: 1 Row: 1 Column: 1 X: -1291.67 Z: 450.87
Apply edit Undo edit Re	

Remove

On this tab you can simply select the layer you wish to remove from the preview window using the mouse or you can specify whether the Top or Bottom of the indicated layer is to be removed.



Replace

This tab provides the option to replace either the top or the bottom of a layer with an existing surface (selected from the Data Explorer and using the add button) or at a specified elevation.

Overwrite existing grid Refine Insert Remove Replace Cells Top of layer Push up Bottom of layer Push down Use surface object New surface name Use elevation Indoff m Minimum layer thickness Non 0.10 m	dit layers ayer edit details Script New grid name NumericalGrid_refined	- □ × Viewing Row • 35 € Exaggeration 20 € € 5 € @ *
 Bottom of layer Push down Use surface object New surface name Use elevation 1.00 m Minimum layer thickness 0.10 m Layer: 1 Row: 1 Column: 1 X: -1180.95 Z: 425.04 	Overwrite existing grid	
0.10 • m	Bottom of layer Bottom of layer Use surface object New surface name Use elevation 1.00 m	
		Layer: 1 Row: 1 Column: 1 X: -1180.95 Z: 425.04 Add objects using the Data and Model Explorer tree checkboxes

Cells

This tab provides allows you to make specific edits to a small number of cells. Use the view settings to find the desired cells in a Row or Column view and click on the cell(s) to be edited. Type in the values you wish to use in the new grid.

it layers	taila a						×
vereditde Newgrid		cript			_		
Numerica						Viewing Row	- 12 🖨 Exaggeration 50 🖃 🔎 🔎 🚱 🍑
Overv	vrite exist	ting grid					
Refine	Insert	Remove	Replace	Cells			
	Layer	Row	Column	Тор	Bottom		
•	1	1	32	19.561	11.786		
	1	1	31	19.469	11.837		╋ <u>╋╫╗╗╗╗╗╗╗╗╗╗╗╗╗</u>
	3	1	31	7.9036	-0.269		
Арр	y edit		ndo edit		leset		v: 12 Column: 43 X: 2029.71 Z: 11.50 g the Data and Model Explorer tree checkboxes
							OK Cancel Help

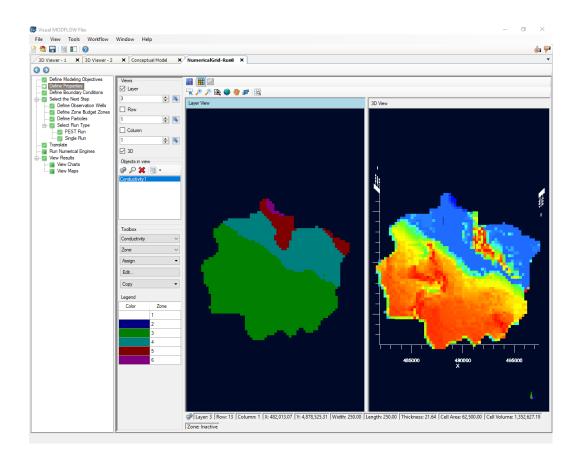
Script

If preferred, you can also make your layer edits by using the Script option. On this tab, you will find the script for any edits you have applied on the Layer edit details tabs allowing you to learn the script language. By making a few changes in the Layer edit details tab (i.e. the options discussed above), you can easily discover the relatively simple syntax of the script. An example of edits to cells and minimum layer thickness settings are shown below. In this manner, advanced users can rapidly incorporate changes to grid layers using external tools such as spreadsheets or custom codes with minimal additional effort:

Edit layers	- 🗆	\times
Layer edit details Script		
<pre>1 Define Grid 2 dx = 40 40 40 40 40 40 40 40 40 40 40 39.9999999999999 40.00000000002 39.999999 3 dy = 40 40 40 40 40 40 40 40 40 40 40 40 40</pre>		
<		>
OK Cance	el Hel	þ

10.4 Define Properties

At this step, you can <u>assign</u>, <u>edit</u>, and <u>copy</u> the flow (and transport) properties for the model. You can also <u>adjust</u> the view/style settings of properties or <u>export</u> the properties.



You can assign properties while viewing either by Layer, Row, or Column; however you cannot edit properties when the 3D subview is active.

Under the Toolbox, use the combo box to select from the available property groups:

• Flow Parameters

- □ <u>Conductivity</u>: includes horizontal conductivity in the X direction (Kx), in the Ydirection (Ky), and vertical conductivity (Kz)
- □ <u>Storage</u>: includes Specific Storage (Ss), Specific Yield (Sy), Total Porosity (Tp), and Effective Porosity (Ep)

□ Initial Heads

□ <u>Vadose Zone</u>: only available/required if using MODFLOW-SURFACT or MODFLOW-2005/MODFLOW-NWT with the UZF package

When transport is included with your model, the following additional property groups may be included:

• Transport Parameters

Initial Concentration Group - one node for each Species
 Species Parameters Group(s) - one or more node for each Species
 Model Parameters Group(s)
 Dispersion

Please Note: the number of Species Parameters and Model Parameters (if any) will depend on what Sorption and Reaction options you have defined in the <u>Define</u> <u>Modeling Objectives</u> step. Please also refer to the <u>Theory</u> section.

For each parameter group, you can choose to render by Zones or by a selected attribute. Based on your selection, the color rendering in the views will change.

The display tools will allow you to switch from discrete cells rendering to color shading/contours (note, this is available only when you do attribute rendering, and not when you are rendering by ZoneID)

	Show/hide grid lines
	Show as cells
2	Show as Surface

At the bottom of the display, you will see in the status bar the position of your mouse cursor in the current view (XY) grid position (Layer, Row, Column), and the Zone ID or attribute value for the selected cell.

For more details on the required flow and transport parameters for each category, please see section: <u>Background on Flow and Transport Properties</u>

Assign

Property zone values can be assigned directly to selected numerical cells using the Assign options from the toolbox.

- **Single**: Select one or more cells with the left mouse button; a small red point will appear over the selected cell
- **Polyline**: Draw one or more polylines to select the desired cells
- **Polygon**: Draw one or more polygons to select the desired cells
- Entire Layer/Row/Column: Selects the currently selected layer/row/column (all active cells)
- Using Data Object: Use data object (points, polylines, or polygons) to select the desired cells

When you use either the Assign/Polygon or Assign/Entire Layer option, the property zone will be assigned to the numerical grid and a corresponding conceptual property zone representation will be created; this is useful when you re-run the Conceptual to Numerical Conversion option for the current (or new) numerical grid.

However, when you use the Assign/Single or Assign/Polyline options, no conceptual property zone is created; please be aware of this limitation should you choose to create a new numerical model from the conceptual model; the property values in this new model run may need to be adjusted.

After you have done the desired cell selections, right click with the mouse to close the shape and select "Finish".

The New Property Zone window will appear as shown below.

ne								Select data object (Drag from Data Tree)
	New							polygon
ne Attributes								Holes in polygons will be ignored
Parameter	Unit	Method		Value		Object	Mapping	O Assign between surfaces
Kx	m/s	Constant	¥	0.0002				V Top surface:
Ку	m/s	Constant	~	0.0002				Bottom surface:
Kz	m/s	Constant	~	0.0002	-			
								✓ Layer 1 ☐ Layer 2 ☐ Layer 3

In the top left, select which zone the selected cells should be assigned to (from the combo box). If you choose an existing zone, the parameter values cannot be adjusted from within this GUI (instead, select the Edit option described above, to adjust parameter values for existing zones.)

Or, click the [New] button to create a new property zone. After doing this, a new zone number will be incremented. Next, select in which layers the new property zone should be generated, by default, your current layer will be selected, however you can include other layers or select all layers.

Lastly, define the "Zone Attributes" for this new property zone in the main grid. There are several "Methods" for defining the attributes, and these include Constant Value and Use Surface (Use 3DGridded Data and Use Shape Data are not applicable for this scenario).

Constant Value

The Constant Value method is selected by default for each parameter in the data input grid and allows you to specify a spatially constant value for the parameter. Replace the default value with a new value.

Use Surface

The Use Surface method allows you use an existing surface data object to define spatiallyvariable attribute values. This is ideal if you have a Surfer .GRD or ESRI ASCII GRD file containing parameter values. Follow the steps below:

Select "Surface" as the method from the combo box. You should then see the button become beside the "Value" column

656

- · From the Data Explorer, select the desired surface data object
- Click the button to insert this data object into the Object field.

Once you are finished, click OK and the new property zone will be created. (note, when you view the Database values for this new property zone, it will show "Distributed Values" since it contains a range of values for this zone, not just a single value).

Use 3D Gridded Data

You may want to define initial concentrations from a .UCN file from a previous transport run. In order to use this option, you must need to import the .UCN file to the project, as a "3D Gridded Data" set. Follow these steps in the section "<u>Import 3D Gridded Data"</u>. Once the file is imported, you select this object when defining the properties.

- Use assign polygon or entire layer, to select the desired group of cells
- Click the [New] button to create a new zone.
- Select "Use 3D Gridded Data" as the method from the combo box.
- You should then see the 🖾 button become activated beside the "Value" column
- From the Data Explorer, select the desired 3D Gridded Data (which contains the imported .UCN file)
- Click the button to insert this data object into the Object field.
- By default, Concentration should be selected in the "Mapping" column (you may need to re-select this from the combo box).
- Once you are finished, click OK and the new property zone will be created.
- You can view the Initial Concentration rendering for the full 3D grid, by changing the rendering type from "Zone" to "Initial Concentration"

Please Note: when you view the Database values for this new property zone, it will show "Distributed Values" since it contains a range of values for this zone, not just a single value)

Edit

Select the Edit button to edit Property zone values after they have been assigned and the Edit property dialog is launched. Here you can select the zone and then you will have the ability to edit any of the cells that are part of the zone.

			Lui	t property					_
dit Cells Script									
lones	Conduc	tivity 🤹 🤇	Calculation						
Zone	L	ayer 🏹	Row	Column	v Kx	: (m/s) 🏾 🏹	Ky (m/s)	Ƴ Kz (m/s)) 7
1			1	3	0.0002		0.0002	0.0002	
2	1		1	4	0.0002		0.0002	0.0002	
3	1		1	5	0.0002		0.0002	0.0002	
	1		1	6	0.0002		0.0002	0.0002	
	1		1	7	0.0002		0.0002	0.0002	
	1		1	8	0.0002		0.0002	0.0002	
	1		1	9	0.0002		0.0002	0.0002	
	1		1	10	0.0002		0.0002	0.0002	
	1		1	11	0.0002		0.0002	0.0002	
	1		1	12	0.0002		0.0002	0.0002	
	1		1	13	0.0002		0.0002	0.0002	
	1		1	14	0.0002		0.0002	0.0002	
	1		1	15	0.0002		0.0002	0.0002	
	1		1	16	0.0002		0.0002	0.0002	
	1		1	17	0.0002		0.0002	0.0002	
	1		1	18	0.0002		0.0002	0.0002	
	1		1	19	0.0002		0.0002	0.0002	

The following buttons are available to assist with your edits:

\sqrt{x}	Expression Builder
	Assign to current cell
	Assign to column
	Apply to selected cells

The Expression Builder, which can be accessed by clicking the \sqrt{x} button, helps you to construct expressions that can include variables and mathematical functions to update property values.

Also available is the Script tab. If preferred, you can make your edits by using the Script option. On this tab you will find the script for any edits you make on the Edit Cells tab allowing you to learn the script language. You can then use the script to "replay" the same edits again.

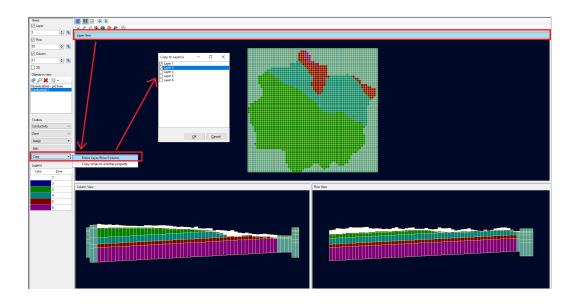
Copy

Property zone values can be copied from the current view to selected numerical cells using the Copy options from the toolbox:

- Entire Layer/Row/Column: copy the properties from the active layer, row, or column view to selected layer(s), row(s), or column(s) based on the active view
- **Copy zones to another property**: copies the property zones for the entire model domain from the current property zone to another selected property type

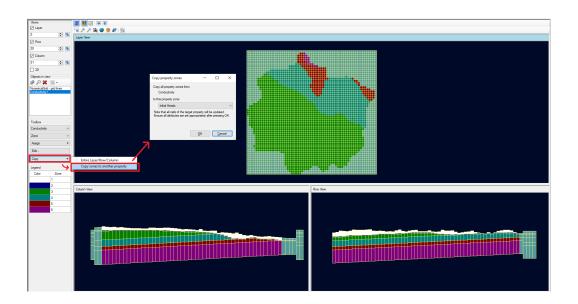
Copy Entire Layer/Row/Column

Select the Copy button and the Entire Layer/Row/Column option to copy property values from the current Layer, Row, or Column based on the active view (i.e. the active view is highlighted in blue) to other layer(s), row(s), or column(s). Note that you can click in a view to make it the active view. Also note that the currently active layer, row, or column will be filtered from the list.



Copy zones to another property

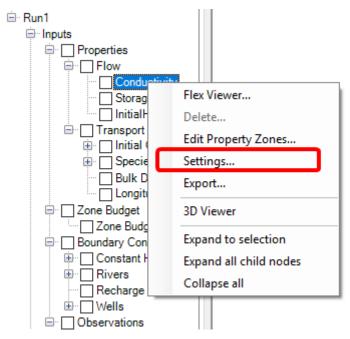
Select the Copy button and the copy zones to another property option to copy the entire set of property zones from the current property type to a different property type. Note that only the zones will be updated, you will need to update the other attributes accordingly.



Adjusting Style Settings

Each group of flow properties exists as a separate item in the model tree, as shown below.

Right click on each node, and select Settings. This will allow you to modify the appearance of each group of flow properties.



In addition, each property group can be added to a stand-alone 3D view; to do this, right click and select 3D-Viewer.

The 2D Colors and Contour line settings can be adjusted. For more details, see <u>Color and</u> <u>Contour settings</u>

Export Properties

Any of the model properties can be exported to a shapefile; see Export for more details.

10.5 Define Boundary Conditions

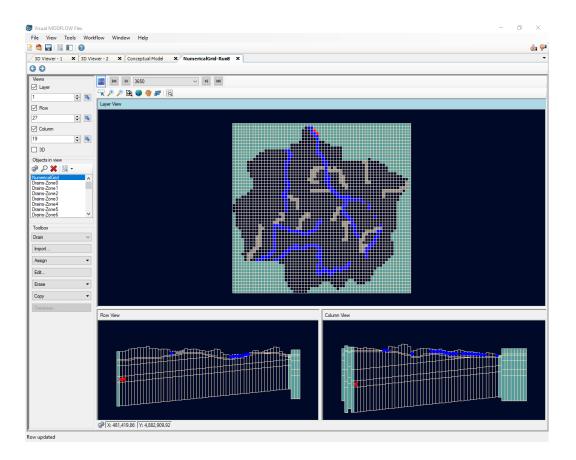
At the Define Boundary Conditions step, you can define and edit the various boundary conditions for your model using one of the following features:

- Import
- Assign

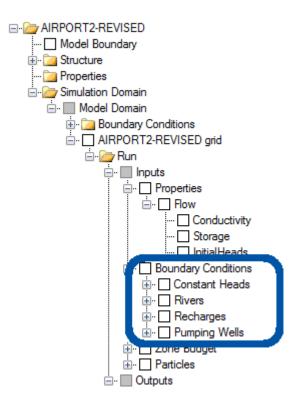
- Edit
- Erase
- Copy
- Database
- Visualizing Boundary Conditions & Style Settings
- Exporting Boundary Conditions
- Boundary Condition-Specific Considerations
 - o Pumping Wells
 - o <u>Head-Dependent Flux Boundary Conditions and Conductance</u>
 - o <u>Recharge and Evapotranspiration</u>
 - o Surface Water

Boundary conditions can be edited in the Layer view as well as in the Row or Column views. Defining and Editing is not supported in the 3D view of finite difference models.

- Under the Toolbox, use the combo box to select from the various Boundary condition types.
- Use the same tools as described in the previous step to manipulate the views.



Each boundary condition group of cells will appear as its own node in the model tree. You can right click on this to adjust style settings. In addition you can load any group of boundary condition cells into a stand-alone 3D Viewer.



To delete a specific boundary condition cell group, right-click on this node in the tree, and select Delete.

Validation

To validate your boundary condition and verify that there are no warning or errors associated with a boundary condition, right-click a specific boundary condition and select Validate... and if there are any errors or warning you will be provided an option to resolve the issue as shown in the dialog below. This is available for Constant Head, River, General Head, and Drain. The validation process will check to see if the attributes of the boundary condition will place it below the bottom of the cell you assigned it to. Then it will give you options to correct this. If you choose to Ignore the errors you may encounter errors when trying to translate and run your model.

đ	Resolve validation failur	res		-	□ ×
8	Waterloo River - Riverbed bottom is below cell bottom in 1 cell(s).	î	Ignore N	•	Apply
			Ignore Delete invalid cells Assign to appropriate layer	1	
					Close

In general, each of the boundary condition types has the same set of graphical tools on the left-hand toolbar for editing the model boundary conditions. The following is a description of how to use these options. For specific descriptions of the data requirements and data entry options, refer to the sections describing each boundary condition type.

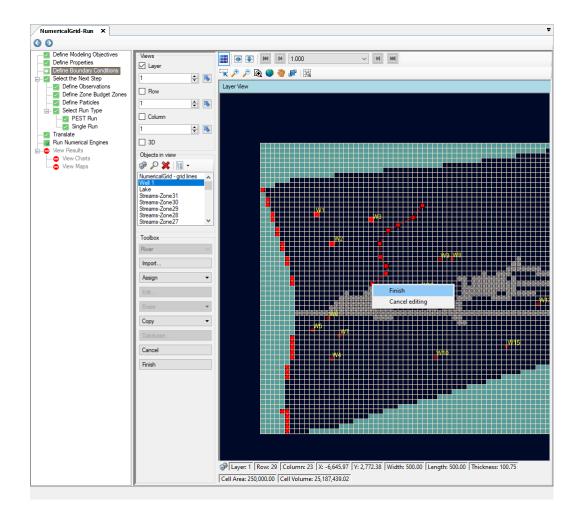
Import

The import button allows you to import boundary condition text files in IJK format. Simply browse to the file and select Open to import the boundary condition. This option is useful when making edits to the boundary condition as described in <u>Edit Attributes in TXT Format</u>.

Assign

The Assign button allows you to assign new boundary conditions. You have options to assign by Polyline or Polygon, by Using Data Object or by Cells. These options are described further below.

• **Polygon** or **Polyline**: Use this option to digitize one or more shapes and assign Boundary Condition attributes to the respective shapes. Use the left mouse button to start drawing. Once you have finished digitizing, double-click or right click with the mouse and select "Finish" to assign the digitized polyline or polygon to the model as shown below.



- Using Data Object: Use this option when you have a polyline or polygon data object already imported into the projects and you would like to use this shape to define the geometry.
- **Cells**: Use this option when you want to select individual cells to assign a boundary condition. For Recharge and Evaporation this can be useful to change only a few cells from one zone to another as the Define Boundary Condition dialog allows you to enter zone numbers.
- RThe Define Boundary Condition attributes window will appear as shown below.

loundary Condition Script		-
Select boundary condition type Constant Head (Type 1) Name: Constant Head 1 Description: Geometry Select a polyline or polygon from Data Explo	 Help Choose the desired boundary condition type from the list, and define a name and optionally, a description. Define where the boundary condition object should be connected on the simulation model domain; this will determine to what model layer the boundary condition will be translated (Top, Bottom, Intermediate). You must then select a polygon or polyline to define the boundary condition geometry. Select the Sides option if you wish to define a boundary condition to the side face of the simulation model domain. For this option, supported boundary condition types are Specified Head, General Head, and Specified Flux 	<u>S</u> how >>
	<< <u>B</u> ack <u>N</u> ext >> <u>C</u> ancel	Help

Provide the desired Name and Description.

chedule Static 🔹 🛤 🔜	Constant He	ad 1 🤹 Ci	alculation		💵 🛤 🖋		
This boundary condition is static. Switch to transient to define a schedule.	Layer	T Row T	Column 🛛	Starting Head (m) 🔽	Ending Head (m) 🔽	Conc001 (mg/L) 🔽	Active 🔽
ransient to define a schedule.	▶ 1	14	1			-1	✓
	1	14	2			-1	✓
	1	14	3			-1	✓
	1	14	4			-1	✓
	1	14	5			-1	✓
	1	14	6			-1	✓
	1	14	7			-1	✓
	1	14	8			-1	<
	1	14	9			-1	✓
	1	14	10			-1	✓
	1	14	11			-1	✓
	1	14	12			-1	<
	1	14	13			-1	> >
	1	14	14			-1	✓
	1	14	15			-1	<
	1	14	16			-1	<
	1	14	17			-1	<
	1	14	18			-1	<
	1	14	19			-1	J

Select Next to proceed.

Define the attributes using the various methods; click Finish when you are done.

This dialog allows you to copy and paste from Excel to make defining (or editing) the attributes easy.

The following buttons are available:

	Assign to current cell (F1)
	Assign to column (F2)
	Apply to selected cells (F3)
P	Interpolate values between selected cells
	Toggle automatic calculation of calculated fields (e.g. river length x river width x river conductivity vs. explicit conductance)

The interpolate option allows you to select 2 cells (rows) and then when you select Interpolate - it will calculate the values for the cells (rows) in between using linear interpolation.

For more details on the options for defining attributes, see <u>Define Boundary Conditions</u> (Attributes).

If your boundary condition is transient switch the schedule drop down to transient to enter your schedule..

Schedule Tra	ansient	- == == =	Constant H	lead 1 🤹 Ca	alculation		II 🗷 🖍		
Start Tin	ne	End Time	Layer	T Row T	Column 🛛	Starting Head (m) 🛛	Ending Head (m) 🏹	Conc001 (mg/L) 🛛	Active 🔽
• 0			▶ 1	40	1			-1	✓
			1	40	2			-1	✓
			1	40	3			-1	✓
			1	40	4			-1	✓
			1	40	5			-1	✓
			1	40	6			-1	✓
			1	40	7			-1	✓
			1	40	8			-1	✓ ✓
			1	40	9			-1	✓
			1	40	10			-1	✓ ✓
			1	40	11			-1	✓
			1	40	12			-1	✓
			1	40	13			-1	✓
			1	40	14			-1	✓
			1	40	15			-1	<
			1	40	16			-1	<
			1	40	17			-1	<
			1	40	18			-1	✓ ✓
			1	40	19			-1	<

You can copy and paste your time schedule from Excel into this dialog to make defining your boundary condition quicker and easier.

By default the Assign to appropriate layer is selected. This means if you enter values for the attributes of a boundary condition (for example the Starting Head) which would place it into another layer - this will occur automatically once you save your boundary condition.

Please Note: When digitizing boundary conditions, Visual MODFLOW Flex will automatically assign these to the appropriate layer, based on the attributes you define. For more details on creating a Wall (HFB) Boundary Condition, please see <u>Define Wall</u> (<u>HFB</u>).

For more details on creating Wells Boundary Condition object, please see <u>Define Pumping</u> <u>Wells</u>.

Edit

When you select the Edit... button you must select a cell containing the boundary condition you wish to edit. The following dialog will appear (similar to defining the boundary condition).

Schedule	Transient	- 📪 📪 😿	Waterloo F	River Calcula	ition					
		o see the attributes of	Layer	T Row T	Column 🔽	Stage (m) 🏼	Bottom (m) 🔽	_COND (m^2/da 🍸	Conc001 (mg/ 🛛	Active 🔽
the cells a	t that time.		1	37	1	16	15.5	125995.02	-1	~
0	к		1	37	2	15.984863	15.484863	144299.38	-1	-
			b 1	37	3	15.969727	15.469727	145214.97	-1	v
	Start	End	1	37	4	15.95459	15.45459	145308.88	-1	~
0		7300	1	37	5	15.939453	15.439453	145072.05	-1	-
			1	37	6	15.924316	15.424316	142129.34	-1	 Image: A state of the state of
			1	37	32	15.594605	15.094605	73762.325	-1	-
			1	37	33	15.587036	15.087036	73362.119	-1	-
			1	37	34	15.575684	15.075684	145694.18	-1	✓
			1	37	35	15.560547	15.060547	145694.18	-1	<
			1	37	36	15.54541	15.04541	144367.65	-1	✓
			1	37	37	15.530273	15.030273	144047.33	-1	✓
			1	37	38	15.515137	15.015137	145944.25	-1	✓
			1	37	39	15.5	15	149762.26	-1	✓
			1	38	7	15.90291	15.40291	144886.16	-1	✓
			1	28	Q	15 887773	15 387773	1///202.05	-1	

The attributes for each cell containing the boundary condition are displayed and can be edited. The cell you selected will be highlighted in the dialog. If you select other rows in the dialog - the corresponding cell will be highlighted in the viewer.

By default the Assign to appropriate layer is selected. This means if you adjust the attributes of a boundary condition (for example the Stage) which would place it into another layer - this will occur automatically once you save your edits.



To view the attributes for Recharge or Evapotranspiration zones, see the Database section below.

Script

If preferred, you can make your boundary condition edits by using the Script option. On this tab you will find the script for any edits you make on the Edit cells tab allowing you to learn the script language. You can re-use the script to "replay" your edits to your boundary conditions.

You can also build expressions using the Expression Builder.

Erase

The Erase button allows you erase the boundary condition assigned to either a single cell or a group of cells. This option is available for all boundary conditions (except Recharge and Evapotranspiration) as well as Walls and Pumping Wells.

Copy

The Copy / Layer/Row/Column option is used to copy all of the boundary data from a selected boundary group to one or more selected model layers, rows, or columns (based on the active view). This option is available for: Constant Head, River, General Head, Drain, Specified Flux and Constant Concentration. When this option is launched, you will see only those boundary condition groups that are in the currently selected layer. Please use caution when copying boundary conditions for an LGR model, as you cannot copy boundary conditions for an user grid to layers in a child grid; you can only copy boundary conditions within the grid in which that it lies (within parent grid layers/rows/columns or within child grid layers/rows/columns).

Copy to layer ×
Select boundary group(s) to copy
Copy all/selected groups
River 1 River 2
Select target layer(s)
Select All Layers
Layer #2
Layer #3
<u>O</u> K <u>C</u> ancel

Database

The Database button becomes active when you select either Recharge or Evapotranspiration for the Boundary Condition type. This will load the zone database window as shown in the following figure.

*		Recharge Attri	bute Info	- 🗆 ×
	Zone	Color	Rate	Ponding Depth
•	1		Undefined	0
	2		2.5	0
			(OK Cancel

In this grid, you can modify the values for existing zones.

Specifying Active/Inactive Time Periods

For Constant Head, River, Drain, General-Head, and Specified Flux, you can disable selected Time Periods by removing the check marks from the Active column (see below), which "turns off" the boundary condition for that particular Time Period. The corresponding package will have no attributes defined for those cells covered by that boundary condition, for that specific stress period. For Recharge and Evapotranspiration zones, you can define a zero rate for those cells in those time periods.

Display

By default, Visual MODFLOW Flex uses the following color scheme for Boundary Condition Cells

Boundary Condition Type	Color	
Constant Head		Red
River		Blue
General Head		Green
Drain		Grey
Lake		Light blue

Recharge	/////	Varies (zone based)
Evapotranspiratio n	////	Varies (zone based)
Unsaturated Zone (UZF)	/////	Varies (zone based)
Seepage Face		Bright Blue
Specified Flux		Beige
Time Varying Material		Orange
Wall (Horizontal Flow Barrier)		Olive
Wells		Light red

Adjusting Style Settings

The style settings of some of the Boundary condition cells

Right click on the desired Boundary condition cell group from the model tree and select 'Settings'.

The Settings dialog will appear; the settings are similar to described in **Points**.

Exporting Boundary Conditions

The boundary condition cell locations (and attributes) be exported to shapefile; see <u>Export</u> for more details.

Boundary-Condition Specific Considerations

Since each boundary condition is intended to simulate different processes, there are functions/behaviors that are unique to certain boundary condition types. For more information on each boundary condition type, please refer to the Boundary Condition <u>Theory</u> section.

Pumping Wells

Pumping Wells are treated differently than other boundary conditions and are pseudoconceptual boundary conditions that are not tied directly to the finite difference grid. To edit a well set:

- Select "Well" from the Boundary Condition list.
- Be sure you are in the correct layer where your well is screened.
- Select [Edit >] Single from the toolbox.
- Select the desired well cell.

😂 Edit	Wells										- 🗆 ×
Well Obje	ct Name: We	ls			Well	Model: WEL ~	Data To	Display Active Well: <none></none>			Display Format Elevation
							Screen	S			 Measured Depths
Vertical					Find:						
Well He	ads						Screen	s			
+ 🖘	🛤 🗱 🖷						🔶 🗄	i 🖦 🗱 🖄 💼			
								ID	Top (ft)	Botton	1 (ft)
	Name	х	Y	Zmax	Zmin	Active	•	Screen0	1055	630	
 	PW01 PW02	17500 22500	27500 27500	1055	630 530						
	PW02 PW03	17500	32500	1046	650						
	PW03 PW04	22500	32500	1052	540						
	PW05	17500	32500	1058	650						
	PW05	22500	37500	1068	570						
	PW07	17500	42500	1083	600			w as Relative Times			
	PW08	22500	42500	1072	550			ig Schedule			
	PW09	17500	47500	1077	600			i 🛶 💥 🖄 💼			
	PW10	22500	47500	1073	550			Start	End	Rate (ft^3.	/s)
		22300	47300	1075	550			1/1/2000 12:00:00 AM	1/1/2050 12:00:00 PM	-10	
								1/1/2050 12:00:00 PM	1/1/2100 12:00:00 AM	0	
										Apply	OK Cancel

• You will see a window similar to the one below:

Please Note: if you make edits to the well pumping rates in this screen, these changes are not propagated back to the raw (original) wells data object in the Data Explorer.

For more information about wells, please refer to the <u>Editing Wells</u>, <u>Well Data</u>, and <u>Theory</u> sections.

Head Dependent-Flux Boundary Conditions - Default Conductance

For Drain, River, General Head, and Lake boundary conditions, you will find an options to **Use Default Conductance** within the Define Boundary Condition dialog.

This allows you to enter attributes more easily measured and have the conductance calculated for you. For example, when assigning a River using a polyline (digitized or data object), you need to provide the River width, Riverbed thickness and Riverbed Conductivity - and the Conductance will be calculated for you based on these fields and the length of the polyline that intersects each cell.

3							Define	Boundary Conditio	n					×
Soundary Condition Script														
chedule	÷ Riv	/er 1	🏠 C	alculation			🗉 🥓 📳 Use de	fault conductance						
This boundary condition is static. Switch to transient to define a schedule.		Layer		Row 🛛		Stage (m) 🏼 🗸	Bottom (m) 🔽	_COND (m^2/day) 🔽	Conc001 (mg/L) V	River Width 🛛	Riverbed Thick 😙	Riverbed Conductivi 😙	Active	
		· 1			3				-1				-	
utilite a sonodale.		1			3				-1				-	
		1		16	3 4				-1				-	
		1							-1				v	
		1		15	4				-1				~	
		1		15	5				-1				-	
Assign to appropriate layer														

If you unselect the **Use default conductance** button, you will need to specify the Conductance values explicitly:

hedule	River 1 🏠 🤇	Calculation		HE C		🖋 📳 Use det	fault con	ductance							
his boundary condition is	Layer		Y	Column	V	Stage (m)	V	Bottom (m)	V	_COND (m ² /day)	V	Conc001 (mg/L)	V	Active	,
static. Switch to transient to define a schedule.	•	18	3								-1			✓	
cilite a scriedule.	1	17	3								-1			✓	
	1	16	3								-1			✓	
	1	16	4								-1			•	
	1	15 15	4								-1			v	
	1	15	5								-1			✓	

Recharge and Evapotranspiration

Recharge and Evapotranspiration have additional settings for rendering the cells by either ZoneID or Rate (either Recharge or Evapotranspiration). To access these settings, right-click on the Recharge (or Evapotranspiration) node in the model tree and select Settings. The following dialog will appear:

eral	Colors			
	Select Data			
е.	Attribute		Max: 175.0000	
eneral lors	Rate	•		
DIOIS			Min: 75.0000	
	Color Classification			Max: 175.000
	Use Project Color Pa	alette Show Project Pale	tte	
	Туре	Classes		
	Stretched	Number of Class	es 8	
	Ŭ	0		
	Classified	Equal Intervals		
	Color	Value	Label	
	255, 0, 0	175		
	255, 146, 0	160.714285714286		
	227, 255, 3	146.428571428571		
	118, 255, 15	132.142857142857		
	64, 255, 83	117.857142857143		
	64, 255, 208	103.571428571429		
	40, 149, 246	89.2857142857143		
	8, 8, 255	75		

From the tree on the left side of this window, select Colors under Style/Recharge. In the main window, under "**Attribute**" you can then change this between Zone or Rate; as you change this, the color range in the grid will refresh. Upon clicking Apply or OK, the 2D/3D views will be refreshed.

Surface Water (SFR2)

The Surface Water workflow only includes the option to "**Edit...**" the boundary condition. Selecting the "**Edit...**" option will launch a new Surface Water workflow or the existing workflow if one was previously created. Since the workflow includes topology data (i.e. the interconnections) of surface water features, there can only be a single Surface Water workflow per model run. The Surface Water workflow is described in detail in the <u>Surface</u> <u>Water workflow</u> section.

10.5.1 Edit Attributes in TXT Format

In certain cases, it may be helpful to export your boundary condition to a text file and make edits to the exported file and then import the boundary condition back into Visual MODFLOW Flex.

You can find this option by right clicking on your individual boundary condition in the Model Explorer:

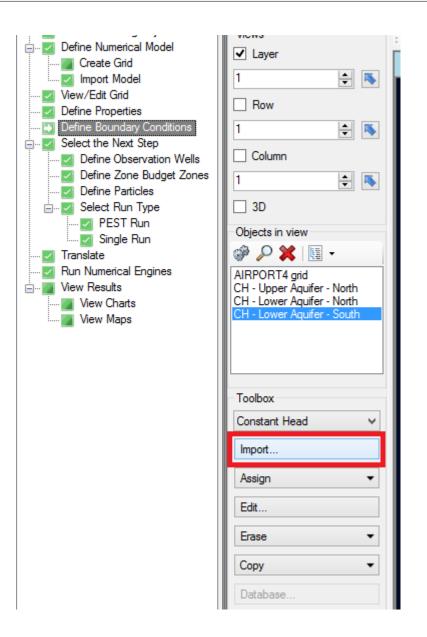
 Simulation Domain Model Domain Image: Image: I					
i⊟- Inputs					
Properties					
Boundary Conditions					
⊡ recharge ⊡ I Constant Heads					
CH - Upper Aquif	or North				
CH - Lower Aquit					
CH - Lower Aqui					
⊡ Rivers	Delete				
	Validate				
	Ement				
Zone Budget	Export				
Zone Budget	Show Time Horizon				
Particles	Settings				
Forward Particles	Settings				
Observations	3D Viewer				
Concentration Obser					
Outputs	Expand to selection				
E Flow	Expand all child nodes				
···· 🔄 Heads	Expand an child hodes				
··· Drawdown	Collapse all				
···· Fluxes					
Indator Table					

You will be provided with a dialog to save the boundary condition as a .txt file. When working with regular (finite difference) grids, the cell index format will be I,J,K while working with unstructured (USG) grids, the cell index format it will be ordered by ID.

You can then make your edits within the .txt file and when you are done import the boundary condition back into Visual MODFLOW Flex.

You will find the import option within the Numerical Workflow at the Define Boundary Condition step.

675



Be sure to select the correct boundary condition type from the drop down before attempting to import the boundary condition file.

10.5.2 Pumping Wells

Visual MODFLOW Flex provides an improved approach and interface for working with pumping wells in the conceptual and numerical model. Visual MODFLOW Flex follows a logical approach of defining the well rate over the entire well, independent of the numerical grid. With this "conceptual" approach, a single well can contain multiple screens, fully penetrating screens, or partially penetrating screen intervals over the depth of the wellbore. Pumping wells are defined at X,Y, and Z co-ordinates, and not assigned to specific grid cells.

This provides flexibility in changing the numerical grid and the ability to readily use well locations (points) as grid node generators for MODFLOW-USG.

Pumping well data are shared between the conceptual and numerical models so that modifications to the conceptual model will translate into the numerical model. Pumping wells are presented in an easy-to-use view showing the well location, screen geometry, and pumping rates. Since the rate is assigned to the entire well, you don't need to worry about figuring out how much discharge is proportioned to each model layer; Visual MODFLOW Flex does this calculation for you automatically. For details on how well rates are calculated for the .WEL package, see the section <u>Calculation of Well Rates</u>.

In addition, if you are running a transport simulation, point source concentrations for an injection well are defined/edited on a per well level, an approach that more closely represents actual field conditions.

Further improvements to wells that will enhance the "ease-of-use" include:

- Dynamically selecting a <u>well model</u> for each well set (See the <u>Theory</u> section for a description of each model).
- Importing pumping schedule data using relative times (starting at 0 days) or using absolute dates (eg. 04/22/2015).
- Setting individual wells as active/inactive in the database view, and having this setting translated to the appropriate well package
- Adding one or more new wells with the click of a mouse
- Visualizing the well screen in cross-section view (by row/column), and in 3D view
- Flexibly labeling and rendering wells and their components (e.g. well path and screens) in 2D and 3D.
- Displaying the well name in the appropriate well package, to correlate the conceptual well to specific MODFLOW grid cells.

Creating a New Wells Object

In the Data Explorer

Well Objects can be created in the Data Explorer by <u>importing wells</u> or you can create a <u>new</u> <u>well object</u> by right-clicking in the Data Explorer, selecting the option Create New Data Object, and selecting Well Set.

🐯 Create New Data Object	\times
Data Type *	
Well Set	\sim
Data Name *	
Well Set1	
OK Cancel H	lelp

🐯 Sp	readsheet										- [- ×
Well Ot Non-V	oject Name: Non	-Vertical	Find:	Model: MNW1		Screen	s ation Points	tive Well: <no< th=""><th>ne></th><th></th><th>Display Forma Display Forma Display Forma Display Forma</th><th>n</th></no<>	ne>		Display Forma Display Forma Display Forma Display Forma	n
	Heads	Ē				Screer	is 1 🛶 💥 1	à 🛱				
							ID		Top Depth (m)		Bottom Dept	n (m)
	Name	Х	Y	Zmax			HS1		203		503	
•	H1	461420.141	4905983.349	242			HS2		1003		1403	
	H2	462176	4906072	242								
						Pumpi	ng Schedule		erence Time 9/1	8/2002 4 Param]
Well	Path								Rate		Paramete	Value \land
-	🖩 🛤 💥 🗐						Start	End	(m^3/d)			0.15
							0.000	3650.000	-100	ľ		
	ID	× (m)	Y (m)	Z (m)	^							0.2
	1	461420.141	4905983.349	242							KSkin	0.001
	2	461420.141	4905983.349	225							В	0
	3	461427.12	4905993.719	212							C	0
	4	461434.098	4906004.089	206							CWC	0
	5	461448.056	4906024.83	201	~					<	I	> ×
,						p			Apply		ОК	Cancel

In a Conceptual Model

- Select a <u>Conceptual Modeling Workflow</u> tab (from the list of active viewers/workflows across the top of the main window)
- Go to the <u>Defining Boundary Conditions</u> step (as shown below)

Svisual MODFLOW Flex - [Conce	nceptual Modeling Tutorial]	- σ ×
File View Tools Workflow	Now Window Help	
2 🧐 🔚 🔢 🗊 🖉		💩 🌳
	Conceptual Hodel 1 ×	=
Data	00	
Data Data	Chef Model Codes Code Deter Conceptual Model Deter Conceptual Model Deter Conceptual Model Deter Conceptual Model Deter Model Structure Deter Mod	
Conceptal Model 1 Model Bondary Model Bondary Hostoria Hostoria Conceptal Hostoria Hostoria Conceptal Hostoria Model Domain Model Domain Model Domain	A work finds Beams days	

- Select Define Pumping Wells. A Create Well Boundary Condition window will appear; the layout is identical to what is shown in the section above for creating wells in the Numerical Model.
- Enter a name for the wells
- On the Data tree, locate the "raw" pumping wells object that you imported into the project
- Click once on the caption for this wells object to select it.
- Drag the wells into the empty text box under "Select Raw Wells Object".
- Release the mouse button
- The list of wells will appear in the window
- Verify that the new wells object contains the correct values, and if necessary make the appropriate corrections. If your previous wells object contained species concentrations for a transport run, then re-assign these now.
- Click OK to complete the process.
- A new item will appear on the Model Explorer under Simulation Domain / Model Domain / Boundary Conditions / Wells
- Once the new wells object is created, you can edit the attributes by right-clicking on the Wells object from the Model explorer under Simulation Domain / Model Domain / Boundary Conditions and selecting Edit Boundary Condition from the menu as shown below.

Model Explorer	
Conceptual Model 2	
Well 1	Delete
	Edit Boundary Condition
	Export
	Settings
	2D Viewer
	3D Viewer
	Expand to selection
	Expand all child nodes
	Collapse all

In a Numerical Model

- Select the Numerical Model workflow tab (from the list of active viewers/workflows across the top of the main window)
- Go to the Define Boundary Conditions step
- Under Toolbox, choose "Wells" from the list of available boundary condition types

• Select Assign / Using Data Object; as shown below:

Toolbox		
Wells	~	
Edit	•	
Assign	•	Wells
		Using Data Object

• The following window will appear:

A	dd Wells							
	bject Name: Well				Well	Model: WEL ~	Data To Display Active Well: Screens	Data To Display Active Well: <none></none>
Select	Raw Wells Data Ob	iject or Drag & [Jrop					
Vertic	al				Find:			
	Heads						Screens	Screens
÷	日本メリー	1					+==×==	十四月X 市自
	Name	X	Y	Zmax	Zmin	Active		
	Name	~	1	Zmax	Zmin	Active		
							Show as Relative Times	Show as Relative Times Reference Time 9/8/2002 4:33 PM
							Pumping Schedule	Pumping Schedule
							中国美义的前	十四月×16

- Enter a name for the wells
- On the Data tree, locate the "raw" pumping wells object that you imported into the project
- Click once on the caption for this well to select it.
- Drag the wells into the empty text box under "Select Raw Wells Object"
- Release the mouse button

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• The list of wells will appear in the window; an example is below

🐯 Ar	dd Wells											- 🗆 ×
Select	bject Name: Well 1 Raw Wells Data Obj VMod Imported Wel	ect or Drag & Drop			Well Mo	del: WEL 🗸	Data To Screen	o Display Active We Is	ell: <none></none>			Display Format
Vertica	al				Find:							
Well	Heads						Scree	ns				
d	👎 🗰 🗱 🐘 🖡	1 1					+ 8	🖬 🛤 🗶 📾 👔				
								ID		Top (m)		Bottom (m)
	Name	х	Y	Zmax	Zmin	Active	►	Screen0		200.89		124.08
►	Underwood #1	461356.999	4906113	244.62	0							
	Scott Point #1	456269.952	4911659.032	178.93	0							
							Pumpi	ow as Relative Times ng Schedule		e Time 9/8/2002 4:33		
								Start	B		Rate (m^3/d)	Conc001
							P	0.000	36	50.000	-29.6	0
											Apply	OK Cancel

- Review the well data, then click OK to complete the process.
- A new item will appear on the Model Explorer under Run/Inputs/Boundary Conditions/Wells, and the new wells should appear in the Flex viewer. If you are viewing by layer, you may need to scroll to the appropriate layers to see the new wells in those screened intervals

Please Note: Creating a new wells object in a numerical model will also create a distinct copy in the corresponding parent Conceptual Model.

- Once the new wells object is created, you can edit the attributes by selecting Edit/Well from the toolbox, and select any well in the numerical model.
- Verify that the new wells object contains the correct values, and if necessary make the appropriate corrections. If your previous wells object contained species concentrations, then re-assign these now.

Options for Wells in the Numerical Model

When you are working in the numerical model, there are three options for adding wells to your model at the define boundary conditions step:

- Assign / Wells
- Assign / Using Data Object
- Edit...

Assign / Wells

Allows you to point and click at locations in the grid (in the current layer) to define one or more well locations. This option is useful if you want to add just a few wells with a simple schedule, and do not have this data already in an Excel file.

- · Select the desired model layer where you want to add a well
- Choose Assign/Wells
- Using the left mouse button, point and click at the desired location.
- When you are finished, click on the "Finish" button on the Toolbox (this can be found under the "Assign" option), or right-click anywhere in the layer view of the grid and select "Define Attributes".
- In the case where a wells object already exists, the following window will appear: (if there are no wells in the project, then the "Edit Wells" window will appear as explained below.

۲	Select Numerical Well Object	-		×
۲	Select an existing numerical well group			
	Well 4			~
0	Create a new numerical well group			
	ОК		Can	cel

- The newly created wells can be added to an existing wells object (new conceptual wells only!) or you can add these wells to a new wells group. This scenario is useful if you want to categorize and distinguish wells in your model (for example separate injection or pumping wells, private vs. public supply wells, etc.)
- Click OK
- The "Edit Wells" window will appear; in this window you can define the screen geometry and pumping schedule. When you add a well with the click of a mouse, the default screen that is created will be fully over the layer thickness; the well Z max will be top of layer 1 and the well Z min will be the bottom of the bottommost layer.
- Click OK to finish creating the wells.

Assign / Using Data Object

Allows you to create a pumping wells object by using an imported wells object as the data source.

- Select the Numerical Model workflow tab (from the list of active viewers/workflows across the top of the main window)
- Go to the Define Boundary Conditions step
- Under Toolbox, choose "Wells" from the list of available boundary condition types
- Select Assign / Using Data Object; as shown below.

Toolbox Wells	
Edit •	
Assign 👻	Wells
	Using Data Object

• The following window will appear:

😻 Add Wells			
Well Object Name: Well 1 Select Raw Wells Data Object or Drag & Drop	Well Model: WEL ~	Data To Display Active Well: <none> Screens</none>	Display Format Elevation Measured Depths
Vertical	Find:		
Well Heads		Screens	
+ == = × ≥ 6		- = = × = =	
Name X Y Zmax	Zmin Active		
		Show as Relative Times Reference Time 9/8/2002 4:33 PM	
		Pumping Schedule	
		+===X % &	
			011
		Apply	OK Cancel

- Enter a name for the wells
- On the Data tree, locate the "raw" pumping wells object that you imported into the project
- Click once on the caption for this well to select it.
- Drag the wells into the empty text box under "Select Raw Wells Object"
- Release the mouse button
- The list of wells will appear in the window; an example is below

	Add							D . T	Display Active V					— □ × Display Format
		t Name: Well 1 w Wells Data Obje	ct or Drag & Drop			Well Mod	el: WEL 🗸	Screen:		vell: <ivone></ivone>				Elevation
		Nod Imported Wells												Measured Depths
Ver	tical					Find:								
W	ell He	ads						Screen	s					
4		🖦 🗶 🐘 🗈						÷ =	🖦 🗙 🐘 🗈					
Г									ID		Top (m)		Bottom	(m)
		Name	х	Y	Zmax	Zmin	Active	•	Screen0		200.89		124.08	
	•	Underwood #1	461356.999	4906113	244.62	0								
		Scott Point #1	456269.952	4911659.032	178.93	0								
								Pumpir	w as Relative Times g Schedule I 📪 💥 🖹 👘		Time 9/8/2002 4:33			
									Start	En		Rate (m^3/d)		Conc001
ш									0.000	365	60.000	-29.6	(
												Apply		OK Cancel

• Review the well data, then click OK to complete the process.

<u>Edit...</u>

Allows you to add a well by entering information directly in the Well Data table.

- Select Edit...
- Clicking on a well in the well group to which you wish to add a well
- Click the " button to add a well
- Add the required information in the well head/path, screen, and pumping schedule tables.
- · Repeat for each well you wish to add
- Review the well data, then click OK to complete the process.

Accommodating Wells with Different Start Times

If you choose a wells data object that contains wells that start at different times, then you will receive a warning when attempting to use this object to create pumping wells; an example is shown below:

Pumping Schedule Modifications	×
The pumping schedules do not all start on the model start date (10/5/2005). The following wells schedules were truncated: Mildmay 1 The following wells schedules were padded with a zero-rate interval: Mildmay 2	
Copy Ok	

The following validations are done:

- 1. The pumping well start date must occur on or after the model start date; any wells with a pumping schedule before the start date will be truncated (cut-off)
- 2. All wells must start at the same start date, and this must be the model start date; in practice, this may not always occur, so VMOD Flex will automatically insert pumping rate of 0 for all wells that do not start at the model start date.

Edit Wells

- Browse to a layer that contains a well; it will appear as a point (colored pink)
- Select Edit/Single
- Click on a Well in the layer view
- The Edit Wells window will appear as explained above.
- Make the desired edits then click OK to apply the changes.

Wells can be set as active/inactive for the simulation; use the "Active" column in the Wells grid to set the appropriate option; wells that are set as Inactive will not be translated to the .WEL package.

Transport Parameters (Species Concentrations)

When you have Transport set as active in the Modeling Objectives, you will have the option to define species concentrations to injection wells; this can be done in the Pumping Schedule, under the "Conc001" column. The injected concentration is assigned to the entire well interval. The default value of -1 is a flag indicating that the injected water does not contain the associated species. One column will be added to the pumping schedule for each

species defined in the Modeling Objectives step - the column header will corresponds to the species name.

Deleting Existing Wells Objects

In the Data Explorer

- Locate the Wells object Data Explorer
- Right click on this object and select "Delete"
- Click Yes to proceed when the warning message appears.

In a Numerical Model

- Locate the Wells object in the appropriate model run in the Model Explorer, under Run/Inputs/Boundary Conditions/Wells
- Right click on this object and select "Delete"
- Click Yes to proceed when the warning message appears.
- Proceed to the next section to also delete the Conceptual Wells from the same project.

In a Conceptual Model

- Locate the Conceptual Pumping Wells object in the appropriate Conceptual Model in the Model Explorer under Simulation Domain / Model Domain / Boundary Conditions / Wells
- Right click on this object and select "Delete"
- Click Yes to proceed when the warning message appears.

Exporting Well Objects

The pumping wells can be exported to a comma separated value (CSV) file; right click on the Model Explorer and select "Export"; a CSV file will be generated which can be loaded into a text editor or Excel.

10.5.3 Theory

A discussion on how boundary conditions are conceptualized and parameterized in Visual MODFLOW Flex can be found <u>here</u>.

Steady-State vs. Transient Flow Boundary Conditions

For transient simulations, MODFLOW requires the time element of the boundary conditions to be defined using Stress Period "counters" as opposed to using "real" times. As a result,

each time interval for a transient model must be determined in terms of Stress Periods before any boundary condition data is defined. Unfortunately, accommodating this format is quite tedious because the data collected for parameters such as rainfall and groundwater recharge don't always follow the same time schedules as data collected for other boundary conditions, such as well pumping rates and surface water levels. This approach also makes it difficult to utilize raw field data collected and recorded in terms of real times.

In Visual MODFLOW Flex, a Time Period is similar to a Stress Period, but with two important exceptions:

- 1. A Time Period is defined using real times and real time units, and
- 2. Each boundary condition grid cell may contain different Time Periods

The advantage of this approach is the ability to clearly see the magnitude of time for each Time Period (as opposed to interpreting data such as "from Stress Period 1 to Stress Period 2"), and it facilitates more convenient methods for importing raw data from different boundary condition types.

Each group of boundary condition grid cells requires a minimum of one Time Period of data containing a Start Time, a Stop Time, and a complete set of data for the selected boundary condition type (the required data for each boundary condition type are described later in this section). For steady-state simulations, Visual MODFLOW Flex requires data for only a single Time Period, while for transient simulations, Visual MODFLOW Flex can accommodate an unlimited number of Time Periods.

For steady-state simulations, the Stop Time value is irrelevant because the term "steadystate" indicates that the model results are not changing with time. Therefore, a Stop Time value of 1 time unit is commonly used. However, if the model is going to be used to evaluate a transient simulation in the future, it is probably a better idea to give it a more realistic value corresponding to the potential time frame of interest.

If a steady-state simulation is run using a model containing transient boundary condition data, only the data from the first Time Period of each grid cell will be used for the steady-state conditions. Furthermore, if the boundary condition consists of starting and ending values (e.g. starting head and ending head for constant head boundaries), the starting value will be used.

Incomplete Boundary Condition Schedules

If the defined period for a boundary condition in a transient model is of a shorter duration that the model itself, Visual MODFLOW Flex will assume that the boundary condition does not exist for the remaining duration. For example, a transient model is run for 10 years, and the recharge boundary condition is defined only for a period up to 7 years, Visual MODFLOW Flex will assume this boundary condition does not exist (i.e. recharge = 0) for the remaining 3 years of the simulation.

The exceptions to this rule are the Constant Head and Constant Concentration Boundaries, which must be defined for the entire simulation.

Steady State Simulations

For a steady-state simulation, a minimum of one active grid cell in the model MUST contain at least one head-dependent boundary condition. Otherwise, the model is indeterminate and the solution will not converge. This head-dependent boundary condition acts as a reference head for all calculations. The head-dependent boundary condition type can be one or more of the following:

- Constant Head (CHD)
- River (RIV)
- Drain (DRN)
- General-Head (GHB)
- Lake (LAK)
- Streamflow-Routing (SFR2)

Transient Simulations

For a transient simulation, the specified initial heads are generally sufficient for a determinant solution.

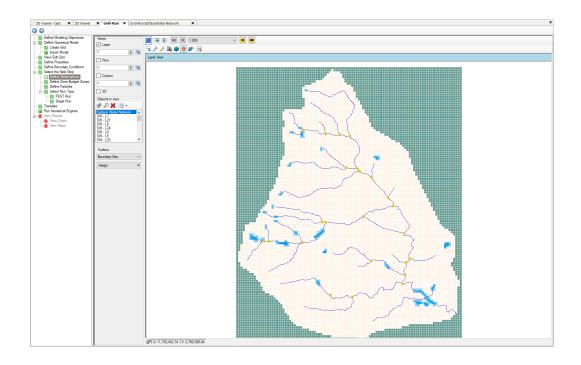
10.6 Define Observations

At the Define Observations step, you can define and edit observation data that can be used to compare your model to historical/expected values for various model outputs and evaluate your model results. The following types of observations can be added to a numerical model:

• Well Observations: heads or concentrations

- **Boundary Obs**: net volumetric flow exchange between the groundwater domain and a specified boundary condition
- Zone Budget Obs: net volumetric flow exchange of groundwater
 - o in/out of a specified zone,
 - $\circ\,$ between a specified zone and another zone, or
 - o between a specified zone and specified boundary condition type
- Surface Water Flow Obs: observations defined in the Surface Water Workflow:
 - <u>Stream (SFR)</u>: stage, depth, outflow, head difference between stream midpoint and associated groundwater cell centroid, flow diverted (diversion segments only), groundwater head, streambed seepage through the unsaturated zone
 - o Lakes (LAK): stage, volume, inflow, outflow

Following a successful model run, assigned observations can be <u>compared</u> to simulated values to facilitate model evaluations including history matching/calibration.



Toolbar

Observations can be defined at the Define Observation step by selecting the type of observation to be defined under the toolbox and selecting the assign option:

• Under the Toolbox, use the combo box to select from the various Observation types:

- o Well Observation
- o Boundary Obs
- Zone Budget Obs
- Surface Water Obs
- Boundary Obs Well Observation Boundary Obs Zone Budget Obs Surface Water Obs

Toolbox

• Then use the Assign button to assign the appropriate object type (described below) defining the observation location.

Well Observations

Well observations include groundwater data collected from wells and piezometers and consist of four components:

- Location: x- and y-coordinates of the sampling point
- **Elevation**: the elevation at which the observation occurred. For monitoring wells, this is typically the midpoint elevation of the screen. For piezometers, this is typically the elevation of the open-ended bottom of the piezometer.
- Time: the time as an absolute date/time or more commonly as elapsed time relative to the model start date
- Value: the value of the observation:
 - Head: the hydraulic head measured in the well or piezometer as top of casing elevation minus depth to water
 - Concentration: solute concentration of the specified species (note that an extra field must be present to define the species)

Prerequisites

To define well observations, you must first have a well data object in the Data Explorer with observation data. You can either <u>import</u> the well observation data or create a new well data object and then add/edit the observation data. The "raw" observation well data can be viewed/edited in the <u>Well Data</u> section.

All other boundary conditions can be fully defined at the Define Observations step; however, you may find that using an imported <u>Time Schedule</u> object in the Data Explorer makes the process significantly more efficient.

Assigning the Well Observations

Once you have imported or created a <u>Well observation</u> data object with heads or concentrations, navigate to the Define Observations step in the numerical model workflow. Below the toolbox, select Well Observation and select Assign > using data object. The Create/Add Well Observations dialog will appear:

😂 Create/Add Well Observations			\times
Select a Well Observation object from the Data Tree:			
$\textcircled{\begin{tabular}{ll} \bullet \\ \bullet $			
Head Obs 1			\sim
○ Assign observations to a new well group			
	ОК	Can	cel

The Create/Add Well Observations dialog contains two controls:

- The assign button (): allows you to specify a well data object with observations in the Data Explorer
- The radio button allows you to specify which observation group the well observation object will be added to in the model tree.

The observation wells should then appear a new node on the numerical model tree on the Model Explorer and any observation well points located in the active layer, row, or column will be also be displayed in the appropriate view(s).

Please Note: If you add Observations that are defined in Absolute times and if some or all of the observation times occur before the model start date defined in the modeling objectives, then you will receive a warning message during creation. These head/concentration observations cannot be included in the numerical model and will be filtered out.

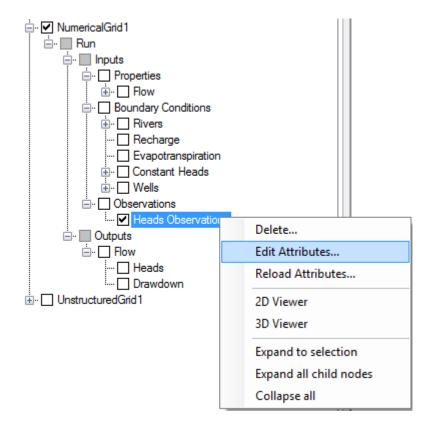
Specifying a Well Observation Group

You will be prompted with a choice to append the observations to an existing well group or create a new well group. Well groups can be used to group observation data into logical sets of data based on a meaningful criteria that may facilitate model calibration, analysis, or evaluation. For example you may wish to group observations by watershed, hydrostratigraphic unit/zone, land use, or property type.

Viewing and Editing Well Observations in CSV Format

Once defined, head or concentration observation data can be viewed/modified in a CSV format:

- Right-click on the Head (or Concentration) Observations node from the Model explorer
- Select "Edit Attributes..." as shown below.



The data contained inside the Observations data object will be displayed in a .CSV file; this should appear in either Notepad or Excel depending on your system configuration; an example is below:

Ę	AutoSave 💽 Of		9 🔒 🗘		16415557-d	670-4dd5-89	a5-7aa300d9	960a8.csv 🝷	۹	Search
F	File Home Ins	ert Draw	Page L	ayout Fo	ormulas I	Data Rev	view Viev	v Develo	per Help	Team
	り・ マ・ Paste ・ ダ	D	ri I <u>U</u> ∽	->[11	~ A^ A`	= =	<u> </u>	č₽ Ξ 🖶 ~	General $\begin{array}{c} \text{General} \\ $	~ 6 9
	Undo Clipboard	L2	F	ont	12	i l	Alignment		Numbe	r 🗔
A	A1 \checkmark : $\times \checkmark f_x$ Well Name									
	A	В	С	D	E	F	G	н	I.	J
1	Well Name	X(m)	Y(m)	Obs. ID	Obs. Elev.	Layer	Obs. Time	Head(m)	Target Resid	dual
2	obore_1/obore_1	131.25	65	Observati	30	1	3.516991	52.6047	1	
3	obore_1/obore_1	131.25	65	Observati	30	1	7.737998	51.54321	1	
4	obore_1/obore_1	131.25	65	Observati	30	1	12.80199	50.67741	1	
5	obore_1/obore_1	131.25	65	Observati	30	1	18.88	49.96522	1	
6	obore_1/obore_1	131.25	65	Observati	30	1	26.173	49.39998	1	
7	obore_1/obore_1	131.25	65	Observati	30	1	34.925	48.97589	1	
8	obore_1/obore_1	131.25	65	Observati	30	1	45.42699	48.67857	1	
9	obore_1/obore_1	131.25	65	Observati	30	1	58.02939	48.48562	1	
10	obore_1/obore_1	131.25	65	Observati	30	1	73.15238	48.37075	1	
11	obore_1/obore_1	131.25	65	Observati	30	1	91.3	48.30856	1	
12	obore_1/obore_1	131.25	65	Observati	30	1	94.81712	48.84876	1	
13	obore_1/obore_1	131.25	65	Observati	30	1	99.03767	49.3166	1	
14	obore_1/obore_1	131.25	65	Observati	30	1	104.1023	49.72452	1	
15	obore_1/obore_1	131.25	65	Observati	30	1	110.1799	50.06768	1	
16	obore_1/obore_1	131.25	65	Observati	30	1	117.4731	50.34068	1	
17	obore_1/obore_1	131.25	65	Observati	30	1	126.2248	50.54399	1	
18	obore_1/obore_1	131.25	65	Observati	30	1	136.7269	50.6845	1	
19	obore_1/obore_1	131.25	65	Observati	30	1	149.3294	50.77394	1	
20	obore_1/obore_1	131.25	65	Observati	30	1	164.4524	50.82594	1	
21	obore_1/obore_1	131.25	65	Observati	30	1	182.6	50.85334	1	
22	obore_1/obore_1	131.25	65	Observati	30	1	186.1171	51.53153	1	
23	obore_1/obore_1	131.25	65	Observati	30	1	190.3377	52.10756	1	
24	obore_1/obore_1	131.25	65	Observati	30	1	195.4023	52.60427	1	
25	obore_1/obore_1	131.25	65	Observati	30	1	201.4799	53.01608	1	

You can use this interface for numerous types of edits/additions:

- Adding a new observation point at a defined XY location
- Change existing data
- Add a new observation time to an existing observation point.

Please Note: the Layer number for the observation point is calculated based on the Obs. Elev; changing the layer number will not change the vertical location of the observation point.

When you are finished with the edits in the .CSV file, you need to save and close this file. Then re-import back the changes into Visual MODFLOW Flex using the steps below:

- Right-click on the Head (or Concentration) Observations node from the Model explorer
- Select "Reload Attributes..."

The modified data will now appear and will be utilized for any charts the next time you translate and run the model.

Defining Boundary Condition Observations

Visual MODFLOW Flex allows you to define observations of net volumetric flows between a specific boundary condition (and its associated collection of cells) and the groundwater flow domain.

Assign Boundary Condition Observations

To define a boundary condition observation data set:

- At the Define Observations step, select the Boundary Obs option in the toolbox
- Click Assign > Using data object...
- The Explorer object select will appear

Explorer object selector	_		\times
Select Numerical BC from explorer			
	Ok	Cano	el

 Select a specific boundary condition object in the Model Explorer (e.g. select "Constant Heads 1" under the Model Explorer tree: Grid > Run > Boundary Conditions >

Constant Heads > Constant Heads 1) and use the assign button () to add that boundary condition object

 Click OK and the Gage Editor window will be displayed allowing you to define the observations

Boundary Condition Observation Types

The gage editor window includes two parts, the left side includes controls to define the observations themselves (i.e. time of observation and the data observed) as described <u>below</u>. In the case of boundary conditions, the only observation type supported is the (net) volumetric flow rate between the groundwater system and the specified boundary condition. By MODFLOW convention, positive values indicate the net flow is from the boundary condition into the groundwater flow system and negative values indicate the direction of flow is from the groundwater system to the specified boundary condition. For example a extractive pumping well and evapotranspiration boundary conditions should produce negative values, while an injection well should produce positive values.

Boundary Condition Observation Spatial Representation

For boundary condition observations, the right side of the gage editor includes the collection of cells associated with the selected boundary condition. You may use the checkboxes and toolbar buttons to toggle which cells associated with the specified boundary condition are included in the observation. The corresponding simulated value will be calculated base on the total net groundwater flow between the groundwater flow cells and the selected boundary condition using information from the output budget file. By MODFLOW convention observations By default, all cells associated with the boundary condition are included.

tor Script												
ge Type Volumetri	c Flow 🝷 ft^	3/d 🛶 拱 👯				Deer Cre	eek-Gage					
Calculation 20		\sqrt{x}				Layer	V			V	Station	V
me	V	Value	V	Target Residual	V	•	3	68 68	50 49			
3		760.6440148		20		_	3	68	45		\checkmark	
60)	878.5767855		20			3	69	48			
9		916.9150734		20			3	69	40			
12	1	896.8315984		20			2	69	46			
15	2	790.7735258		20			3	69	45			
18	2	650.1701356		20			2	69	40			
21	3	503.2321094		20			2	69	43			
24	4	386.7933872		20			2	70	43			
27	4	314.1950949		20			2	70	43			
30	5	325.8821025		20			2	70	42			
33	5	396.4973335		20			2	70	41			
ŧ							2	71	41			
-							2	71	39			
							2	72	39		$\mathbf{\nabla}$	
							2	72	38			
							2	72	38			
							2	72	37			
							2	/3	3/			

Please Note: if the specified collection of cells includes other boundary conditions of the same type, then the affects of these other boundary conditions will be included in the observation as the output budget file produced by versions of MODFLOW lump flow terms for boundary conditions of the same type.

Defining Zone Observations

Visual MODFLOW Flex allows you to define observations of net volumetric flows using ZoneBudget zones.

Assign ZoneBudget Observations

To define a boundary condition observation data set:

- At the Define Observations step, select the Zone Budget Obs option in the toolbox
- Click Assign > Using data object...
- The Gage Editor window will be displayed allowing you to define the observations

Zone Budget Observation Types

The gage editor window includes two parts, the left side includes controls to define the observations themselves (i.e. time of observation and the data observed) as described <u>below</u>. In the case of Zone Budget zone observations, the only observation type supported is the (net) volumetric flow rate. By MODFLOW convention, positive values indicate the net flow is <u>into</u> the groundwater domain of the specified ZoneBudget zone.

Zone Budget Observation Spatial Representation

The right side of the Gage Editor includes the spatial definition of the observation. For ZoneBudget zone observations, the right side of the gage editor includes two dropdown selectors:

- Selected Zone (From): The "from" zone selection allows you to specify the zone where groundwater flows are to be observed.
- Selected Zone (To): The "to" zone selection (shown in red) is optional and allows you to specify a different ZoneBudget zone or a boundary condition type present in the model. If not selected, then the net groundwater flows to all adjacent zone budget zones will be observed.

Gage Type Volumetric Flow • ft^3/d ↓ <t< th=""><th>Gage station name Zone Budget-Gage 3 Selected zone (From): Zone 1</th></t<>	Gage station name Zone Budget-Gage 3 Selected zone (From): Zone 1
Time Value Target Residual Value 31 145.1102643 5 60 112.8110465 5 91 141.8077018 5 121 111.6546235 5 152 55.67374097 5	Zone Budget-Gage 3 Selected zone (From):
Value Target Residual Value 31 145.1102643 5 60 112.8110465 5 91 141.8077018 5 121 1111.6546235 5 152 55.67374097 5	Selected zone (From):
60 112.8110465 5 91 141.8077018 5 121 111.6546235 5 152 55.67374097 5	
91 141.8077018 5 121 111.6546235 5 152 55.67374097 5	Zone I
121 111.6546235 5 152 55.67374097 5	
152 55.67374097 5	
	Select zone (To)
182 69.36806236 5	Zone / Boundary condition
213 102.1205018 5	×
244 148.2311585 5	Zone 2
274 118.2628886 5	Zone 3
305 52.55330493 5	Constant Head NA
335 115.9618202 5	River NA
*	

Defining Surface Water Observations

Visual MODFLOW Flex allows you to define observations of <u>various</u> types of data observed in streams and lakes developed in the <u>Surface Water Workflow</u>.

Assign Surface Water Observations

To define a boundary condition observation data set:

- At the Define Observations step, select the Surface Water Obs option in the toolbox
- Click Assign > Using data object...

- The <u>Surface Water Workflow</u> will open allowing you to create stream reach and lake observation gages using the surface water network <u>tools</u>.
- Once a gage has been created, you can add/edit observation data using the surface water <u>gage editor</u> window.

Gage Editor

The gage editor includes several controls allowing you to define and edit observations. The left side of the panel allows you to define the observations (e.g. time, value, and target residual) while the right side of the panel allows you to define the spatial scope over which the observation(s) apply (e.g. the collection of cells where the volumetric flow is to be measured).

e Type Volumetr	ic Flow - ft^	3/d 🚃 🙀 🙀				Deer Cr	eek-Gage		1		
Calculation 20		\sqrt{x}				Layer	v v		y ⊽ Column	∇ Station	2
ne	γ		V	Target Residual	V	> Layer	3	68	50		
	-		¥		Ŭ		3	68	49	-	-
3		760.6440148 878.5767855		20			3	68	48	-	<
-	0	8/8.5/6/855 916.9150734		20			3	69	48	2	<
9	21	896.8315984		20 20			3	69	47	-	
3	52	790.7735258		20			2	69	46	2	7
	52 32	650.1701356		20			3	69	45	-	1
2		503 2321094		20			2	69	44	-	<
24		386 7933872		20			2	69	43	-	<
24		386./933872 314.1950949		20			2	70	43	2	4
	/4)5	314.1950949 325.8821025		20			2	70	42	2	_
	15 35						2	70	41	-	_
3.	35	396.4973335		20			2	71	41	-	
							2	71	40	2	/
							2	71	39	-	
							2	72	39	-	/
							2	72	38	~	
							2	72	37	~	
							2	73	37	-	1

Observation Schedule

The left side of the Gage Editor dialog includes the following controls for all supported types of observations (boundary conditions, zone budget zones, stream, and lake gages):

- **Gage Type**: allows you to select the type of observation to be measured and associated project <u>units</u>. The stream and lake gages support a variety of observation types as described above and the remaining gages/observation types are limited to volumetric observations. Note that well observations are handled separately using well objects (see above).
- **Toolbars:** the gage toolbars include the following buttons:
 - o 🔤 Add interval: adds an observation time at the end of the table
 - o 🖽 Insert interval after selection: adds an observation time after the selected row
 - Delete selected row(s): deletes selected row(s) from the table

- o 🄹 Clear sort: clears the sort order (if any) on fields in the observation table
- $\circ \sqrt{x}$ Expression builder: opens the Expression builder
- III Assign to column: evaluates the Expression for all cells in the current column
- Assign to current cell: evaluates the Expression for all selected cells in the current column (press and hold SHIFT or CTRL buttons with left mouse clicks to select multiple cells)
- Table: the table in the left hand side of Gage Editor includes three fields:
 - o Time: elapsed time relative to the model start date
 - Value: the value of the observation. Note that positive flow values for volumetric observations follow the standard MODFLOW convention that positive values indicate flow <u>into</u> the groundwater flow system
 - *Target Residual*: the target difference between observed values and simulated results (based on project goals, stakeholder input).
- Load Schedule Object: Selecting this option will allow you to load the data from a time schedule object in the Data Explorer and map fields from the schedule object (using the dropdown selectors) to the value and target residual fields.

Gage schedule field mapping			-		×
Zone Budget-Gage 3					
Gage field	Project unit	Schedule field			
VolumetricFlow	ft^3/d	Value			
VolumetricFlow (Residual)	ft^3/d	Target Residual			\sim
		None			
		Value			
		Target Residual			
			OK	Ca	ncel .:

Observation spatial scope

With the exception of certain stream and lake observations, the observation types apply generally apply over a defined area rather than at a discrete point. As such, the right side of the panel is used to define the spatial extent/scope of the observations that will be used for extracting simulated equivalent values to be compared to the observations. Since the various observation types have differing contexts, the applicable interface is dependent on the type of observation:

- Boundary Condition: allows you to define a specific boundary condition for observations
- **Zone Budget Zone**: allows you to define the primary zone from which flows may be leaving (or entering) and (an optional) secondary zone or boundary condition type to which flows are entering.
- Steam: allows you to define a stream reach for observations (via the <u>gage</u> package)
- Lake: allows you to define a specific lake for observations (via the gage package)

Script

The Script tab allows you to quickly add or modify data based on a script. If you are interested in using the script, try to define a simple gage to observe the structure and add complexity. An example is shown below:

iditor Script		
1 Define Gage BCStation		
2 Name = "Zone Budget-Gage 3" // nam	es containing non-alphanumeric characters must be quoted	
<pre>3 StationScope = None</pre>		
4 ZBPlugin = a678958f-1c0c-416c-9f24-	<u>3a0c87b</u> 8d35c	
5 Selection = Zone		
6 (Observation Scope	
7 ZoneId = 1	observation scope	
8 }		
9 X = 3119.56521739131	La catina	
Y = 3079.22535211267	- Location	
1 Z = 601.535340199951		
2 StationData = 3 GageType = VolumetricFlow	Observation Type	
.3 GageType = VolumetricFlow .4 ObservationSet =	⊢ Observation Type	
.5 005ervationSet =		
6 1155 666.539142372955 30		
1135 000.339142372935 30		
1216 800.681547494757 30		
9 1247 785.600533274997 30		
1277 861.167336965562 30		
1308 828.314825628306 30	Observation Data	
2 1339 833.415712460441 30		
3 1369 798.396213600784 30		
4 1400 600.374244465833 30		
5 1430 582.908905009703 30		
6 1461 492.477152088483 30		
7 1492 395.455497562577 30		

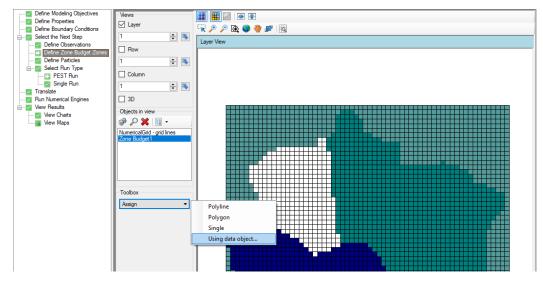
- The header defines the type of observation and (other than the name, which should be wrapped in "quotes") should not be edited.
- The Observation Scope section defines which objects are associated with the observation gage.
- The **Location** section defines where the observation will be rendered in views when displaying residuals
- The **Observation Type** defines which observation data are used. You can specify more than one Observation Type block
- The **Observation Data** includes the set of times, observations, and target residuals for the time above.

Similar to a macro builder, any edits you make on the Edit tab will be reflected at the Script tab. In this way you can experiment with the Gage Editor and learn to build your own scripts.

10.7 Define Zone Budget Zones

ZoneBudget is a USGS program for computing subregional water budgets for MODFLOW ground-water flow models. Within Visual MODFLOW Flex, you can create new zones for MODFLOW-2000 and -2005 models in the numerical model workflows. If you imported a Visual MODFLOW Classic model, you can also view the zone budget zones that were defined in this numerical model.

At the Define Zone Budget Zones step, you can create new zone budget zones by digitizing new zones using Assign Polyline, Polygon, or Point (Single Cell), or by using 2D/3D point, polyline, or polygon shape objects from the Data tree.



Follow the steps below to create new zone budget zones:

Assign

You can assign a set of cells to a specific Zone Budget Zone using the following tools:

Polyline

• Use the left mouse button to start digitizing a polyline over the desired cells. Once you have finished digitizing, click on the Finish button from the toolbox, or right click with the mouse and select "Define Attributes". The following window will appear

Create new zone budget zone	
 Assign to single zone Select zone: 	
Zone 1 New O Create new zones from attribute	
No attributes \checkmark Use integer field values	
Assign to layer Assign to all layers	
Layer 1 Layer 2 Layer 3 Layer 4 Layer 5 Layer 6	
OK Cancel Help	

• Click the New button to assign the selected cells to a New zone; otherwise, you can select to assign cells to an existing zone by selecting the zone from the dropdown list at the top. The selected cells can be assigned to the current layer or multiple layers using the check boxes at the bottom of the window. Once you are finished, click OK.

Polygon

• Digitize one or more polygons, and repeat the steps as described above for Polylines.

Single

• Left-click on one or more cells and a point will appear. Once finished, right-click and select "Define Attributes", and follow the steps as described above for Polylines.

Using Data Object....

• The following window will appear.

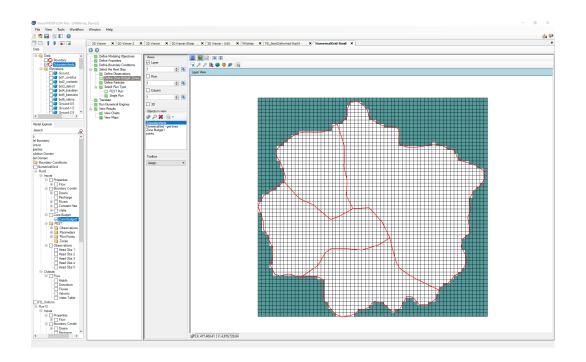
Select geometry object	x
Select a points, polyline or polygon data object]
OK <u>C</u> ancel	

- Choose the desired point, polyline, or polygon data object from the tree.
- Click on the button (under Select Data Object)
- A second window will appear:

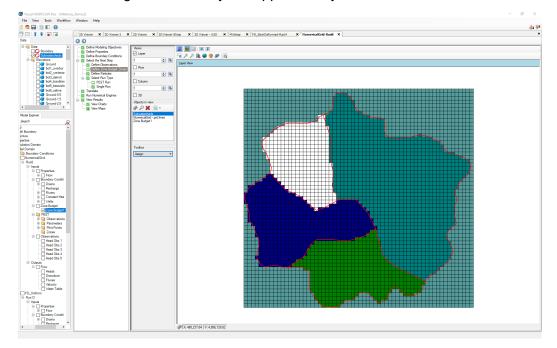
O Assign to single zone	
Select zone:	
Zone 1 Vew	
 Create new zones from attribute 	
Zone 🗸	
Use integer field values	
Assign to layer Assign to all layers Assign to all layers Layer 1 Layer 2 Layer 3 Layer 4 Layer 5 Layer 6 OK Cancel Help	

- Select which zone you want the features to apply to. You have the option to assign the zones to:
 - $\,\circ\,$ An existing zone
 - o A new single zone
 - o Create zones for individual features
 - o Create zones based on feature attributes
- Select the desired model layers where the zone should be applied

A simple example for a polygon data object (red) is shown below:



After the zones are generated, they will appear in layer view:



When the selected shape contains multiple polyline or polygon features, then a new zone will be created for each feature. You can also use an attribute field to select if polygons represent a specify zone. If the attribute field is an integer field, then you can also assign the zones based on the integer values in that field.

10.8 Define Particles

Introduction

Particle-tracking is a useful tool for Groundwater Modelers that provides insights and diagnostics in the modeling process. Two particle tracking engines are supported in Visual MODFLOW Flex:

- MODPATH
- MOD-PATH3DU



MODFLOW-LGR models are not compatible with the particle tracking in Visual MODFLOW Flex

MODPATH

The computer program MODPATH was developed by the USGS (<u>Pollock, 1998</u>) to calculate three-dimensional particle tracking pathlines from steady-state and transient flow simulation output obtained using MODFLOW-2000, MODFLOW-2005, MODFLOW-NWT, MODFLOW-SURFACT, and SEAWAT.

MODPATH uses a semi-analytical particle-tracking scheme. The method is based on the assumption that each directional velocity component varies linearly within a grid cell in its own co-ordinate direction. This assumption allows an analytical expression to be obtained describing the flow path within a grid cell. Given the initial position of a particle anywhere in a cell, the co-ordinates of any other point along its path line within the cell, and the time of travel between them, can be computed. Documentation of the theoretical and numerical implementation of MODPATH are given in Pollock (<u>1998</u>), while source code and input documentation are available at the USGS <u>MODPATH webpage</u>. MODPATH in Visual MODFLOW Flex is not currently compatible with MODFLOW-USG or MODFLOW-LGR.

MOD-PATH3DU

The computer program mod-PATH3DU was developed as part of a collaboration between S.S. Papadopulos & Associates, Inc. (SSPA) and the University of Waterloo (Muffels, et al, <u>2016</u>) and calculates three-dimensional particle tracking pathlines from steady-state and transient flow simulation output.

Similar to MODPATH, mod-PATH3DU uses a semi-analytical particle-tracking scheme based on the linear interpolation of the velocity field within a given grid cell. The major difference is that mod-PATH3DU supports intra-cell velocity field interpolation using the Waterloo method, which is based on a high-order Runge-Kutta scheme and is valid for any prismatic cell geometry. In addition to the flow engines supported above, mod-PATH3DU also supports MODFLOW-USG.

A more thorough explanation of the method is documented by Rhamadhan (2016).

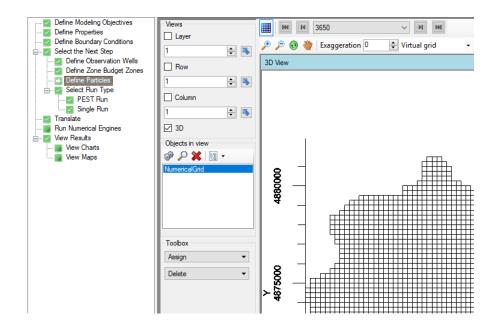
NOTE: mod-PATH3DU is developed/maintained by SSPA (a third party) and is not directly included in Visual MODFLOW Flex. It is available for free via registered download at the SSPA website for mod-PATH3DU.

Visual MODFLOW Flex currently only supports mod-PATH3DU versions 2.12 and later.

Please Note: MOD-PATH3DU version 2.12 currently only supports fully structured grids or unstructured grids with continuous layers. In other words, the lateral discretization must be the same for all layers in the model. The Visual MODFLOW Flex grid generator for Q-Grids does not generate such grids where pinchouts are specified, therefore the use of V-Grids is recommended for conceptual models with pinchouts when using MODFLOW-USG. Version 3, likely to be released in the near future, will support discontinuous layers in unstructured grids.

Working with Particles in Visual MODFLOW Flex

At the Define Particles step, you can create, modify and view groups of Forward and Backward Particles, including those that have been imported from a Visual MODFLOW Classic model.



Assign

You can assign particles using one of the following methods:

Points	
Circle	
Polyline	
Polygon	
Using data o	bject
Using well of	oject

Points...

- First, select the model layer, row, or column where you want the circle to be assigned.
- Select the option [Assign > Circle] from the toolbox.
- Using the mouse, left-click on the Layer, Row, or Column view at the desired locations for the particles.
- Once finished, right-click and select "Finish", or click on the Finish button from the toolbox, and the following window will appear:

Assign P	oints in Layer View	Assign Points in Row or Column Views
Create New Particles	- 🗆 ×	📚 Create New Particles — 🗆 🗙
Particle group name Points Group 1	Particle propagation Forward Backward 	Particle group name Particle propagation Points Group 1 Forward Backward
Select object Assign elevation Specified layers Specified elevation	Release time Beginning of simulation Custom 0	Select object Release time End time Image: Select object Image: Select object Image: Select object ob
	Assign to layer Layer Position Layer 1 Center Layer 2 V	<u>Q</u> K <u>C</u> ancel
	Layer 3 ~ Layer 4 ~ Layer 5 ~	Assign End Time Release time End time O Beginning of simulation
Custom elevations Method Value	e Object	End of simulation Custom O 'Applies only to MODPATH-3DU

The following data inputs will be available:

- Particle group name: A unique name for the particle group
- Select Object: not applicable as you have defined the location of the particles
- **Particle Propagation**: provides the option to select whether the particles will propagate forwards or backwards in time
- Assign Elevation: (layer view only)
 - Specified Layers: the Assign to layer method will be used to assign particles to specified layers as described below

- Specified Elevation: the Custom elevations method will be used to assign particles by elevation as described below
- **Release Time Tab**: provides the option to select when the particle group is released (i.e. tracking is initiated)
 - *Beginning of Simulation*: particles in the group are released at relative model time = 0; this is the default for forwards-in-time particles
 - *End of Simulation*: particles in the group are released at the end of the model simulation period; this is the default for backwards-in-time particles
 - *Custom*: particles are released at the specified (relative) time based on the time units specified in the project settings.
- End Time Tab: provides the option to select when particle tracking is terminated (if the particle has not yet reached an endpoint such as a sink for forwards particles and a source for backwards particles). Note this applies only to mod-PATH3DU simulations
 - *Beginning of Simulation*: remaining particles in the group are terminated at relative model time = 0; this is the default for backwards-in-time particles
 - *End of Simulation*: remaining particles in the group are terminated at the end of the model simulation period; this is the default for forwards-in-time particles
 - *Custom*: remaining particles in the group are terminated at the specified (relative) time based on the time units specified in the project settings.
- Assign to Layer: if the Assign Elevation option is specified layers, this option provides you with a table with entries for each layer where you can assign the particles to the specified layer(s) and whether the particles will be assigned to the layer Top, Center (middle), or Bottom.
- **Custom elevations**: if the Assign Elevation option is specified elevation, this option provides you with following inputs
 - *Method*: Choose from:
 - Constant: a specified constant elevation based on the entered Value
 - Surface: a surface data object from the project explorer (use the blue arrow to choose an item selected in the Data Explorer)
 - Horizon: a horizon object from the model explorer window (use the blue arrow to choose an item selected in the Model Explorer)
 - Water Table: a water table object from the model explorer window (use the blue arrow to choose an item selected in the Model Explorer)
- Click OK when you have finished.

Circle...

A circle of backward tracking particles is typically assigned around a pumping well in order to determine the capture zone for that well.

- First, select the model layer where you want the circle to be assigned.
- Select the option [Assign > Circle] from the toolbox
- Move your mouse cursor to the location where you want the center of the circle to be located (typically on top of a well cell, at the center of the cell). This option is available in Layer View only
- · Left-click once to create the circle
- The "Define Particles Window" will appear

Particle group name		Particle propagation	
Circle Group		O Forward	Backward
Select object		Release time End tim	ne
		O Beginning of simulation	
Particles on circle		End of simulation	
Radius: (m) 10		O Custom	
# Particles 10		0	
Assign elevation		Assign to layer	
Specified layers		Layer	Position
 Specified elevation 		Layer 1	Center
		Layer 2	
		Layer 3	
		Layer 4	
		Layer 5	
		Layer 6	
Custom elevations			
Method	Value	Ol	bject

- Define the Radius for the Circle
- Define the # Particles to be inserted
- Define the Particle Propagation Direction, Assign elevation options, and Release time, as explained <u>above</u>.
- Click OK when you have finished.

Polyline...

- First, select the model layer, row, or column where you want the polyline to be assigned.
- Select the option [Assign > Polyline...] from the toolbox.
- Using the mouse, left-click on the Layer, Row, or Column views to draw the polyline in the desired view.
- Once finished, right-click and select "Finish", or click on the Finish button from the toolbox, and the following window will appear:

Assign Polyline in Layer View

Assign Polyline in Row or Column Views

Particle group name	Particle propagation	Particle group name	Particle propagation
Polyline Group	Forward O Backward	Polyline Group	Forward O Backward
Select object	Release time End time	Select object	Release time End time
\Rightarrow	Beginning of simulation		Beginning of simulation
Particles on polyline	End of simulation	Particles on polyline	 End of simulation
Evenly spaced 10	◯ Custom	Evenly spaced 10	Custom
Drop particle at every	0	O Drop particle at every	0
	Assign to layer		
Assign elevation	Layer Position		
Specified layers	✓ Layer 1 Center ✓		OK Cancel
 Specified elevation 	Layer 2 V		
	Layer 3 V		n End Time
	Layer 4 V	Release time End	l time
	Layer 5 V		of simulation
	Layer 6 V	End of simu	lation
Custom elevations			lation
Method Value	Object	O Custom	
		-	

The following data inputs will be available in addition to those described above:

- Particles on polyline:
 - *Evenly spaced*: the number specified particles will be placed using even spacing along the pathline
 - Drop particle at every: particles will be placed along the polyline using the spacing provided, in project length units
- Click OK when you have finished.

Polygon...

- First, select the model layer, row, or column where you want the polygon to be assigned.
- Select the option [Assign > Polyline...] from the toolbox.
- Using the mouse, left-click on the Layer, Row, or Column views to draw the polygon in the desired view.
- Once finished, right-click and select "Finish", or click on the Finish button from the toolbox, and the following window will appear:

Assign Polygon in Layer View

Assign Polygon in Row or Column Views

Particle group name	Particle propagation	Particle group name	Particle propagation
Polygon Group	Forward O Backward	Polygon Group 1	Forward O Backward
Select object	Release time End time	Select object	Release time End time
\Rightarrow	Beginning of simulation		Beginning of simulation
Particles on polygon	End of simulation	Particles on polygon	 End of simulation
Positioned across a boundary grid of size:	Custom	 Positioned across a boundary grid of size: 	Custom
# Columns 10 🚖	0	# Columns 10 🚖	0
# Rows 10 🜩	Assign to layer	# Rows 10 🜩	
Assign elevation	Layer Position		
Specified layers	✓ Layer 1 Center ✓		OK Cancel
 Specified elevation 	Layer 2 V		
	Layer 3 🗸 🗸	Assig	n End Time
	Layer 4 V	Release time En	d time
	Layer 5 V		of simulation
	Layer 6 V	End of sim	
Custom elevations			ulation
Method Value	Object	O Custom	
		0	

The following data inputs will be available in addition to those described above:

- **Particles on polygon**: particles will be placed on a rectangular grid within the polygon using the specified number of columns and rows
- Click OK when you have finished.

Using Data Object

 Select the option [Assign > Using Data Object] from the toolbox and the following window will appear:

Create New Particles				—	
Particle group name		Particle propa	agation		
Points Group1		Forwar	rd 🔿 E	Backward	
Select object		Release time	End time		
⇒		Begin	nning of simul	ation	
Assign elevation		 End of simulation 			
Specified layers		Custom			
Specified elevation		0			
		Assign to laye	er		
			ayer	Position	
		🗹 Lay	yer 1	Center	~
		Lay	yer 2		~
			yer 3		~
			yer 4		~
			yer 5	_	~
		Lay	yer 6		~
Custom elevations					
Method	Value		Objec	t	
			⊨		
			OK	_	

- From the Data Explorer, select a Points, Polyline, or Polygon data object that represents the features/locations where particles are desired. If you do not have a file containing these features, then you can create and digitize new points, polylines, or polygons using the drawing tools. Refer to <u>Creating New Data Objects</u> for more details.
- Click the button to insert the data object into the input field.
- The window will update and provide the same options as assigning by <u>points...</u>, <u>polyline...</u>, or <u>polygon...</u> as described above based on the input type.

Please Note: In addition specifying the particle elevations by layers or specified elevations, you may also use the elevations of the feature objects

• Click OK when you have finished.

Delete Particles

• [Delete >] By Drawing a Box, allows you to delete just a set of particles. Note that this option will only delete the particle type that is active at that time (either Forward or Backward). Before proceeding with the Delete, be sure you have the desired particle type

layer as active (and visible in the 2D Viewer). To do this, click on \square , and move the desired layer type (Forward or Backward particles) to the top of the layer list. Once complete, select Delete > Draw in a Box, and left click with your mouse to anchor the corner of a box around the selected particles you wish to delete, then draw the outline of the box, and release the mouse button to complete the box. The particles that lie within

that box will be deleted, though only for the current model layer.

- [Delete >] Current Layer deletes all particles (Forward and Backward) in the current layer
- [Delete >] All Layers, deletes all particles in all layers

MODPATH Options

There are several settings for the MODPATH run, which can be define at the "Translate" step. For more details, see <u>MODPATH</u>

10.9 Select Engines

One of the main benefits of Visual MODFLOW Flex is the dynamic integration of all of the numeric engines including:

- Flow: MODFLOW 2000, MODFLOW 2005, MODFLOW-6, MODFLOW-NWT, MODFLOW-LGR, SEAWAT, or MODFLOW-SURFACT (Note that MODFLOW-USG is handled through a separate <u>workflow</u>).
- Transport: MT3DMS, MODFLOW-6, RT3D, SEAWAT or MODFLOW-SURFACT
- Post-Processing: MODPATH, MOD-PATH3DU, and/or ZONEBUDGET

The Single Run workflow step is used to select the Flow and Transport Engines and Post-Processing Utilities you wish to include in the model run. Visual MODFLOW Flex requires you to select a flow engine for a particular run. However, once you have run the flow engine at least once, you can reuse it, as described <u>below</u>. Running a transport engine, a particle track engine, and/or ZONEBUDGET is typically optional.

G	
Define Modeling Objectives	Use a previous flow engine run (if available) Row Engine
Import Model	USGS MODFLOW 2005 from WH V
Define Properties	Run Transport Engine
Select the Next Step	MT3DMS ~
	ZONEBUDGET
🖃 🚽 Select Run Type	Particle Tracking
····· <mark>✓ PEST Run</mark> ·····	MODPATH
Iranslate Iranslate Run Numerical Engines	
in Wiew Results	
View Maps	

The flow and transport engine(s) available for selection are based on the flow and transport options chosen at the the <u>Define Modeling Objectives</u> workflow step as well as the selected grid type. For example, parent/child grids used with MODFLOW-LGR flow models are not currently compatible with any of the transport engines, ZONEBUDGET, MODPATH, or

MOD-PATH3DU. However, model results from an LGR run can be <u>extracted to a standard</u> <u>finite difference subgrid</u> and subsequently run with transport, ZONEBUDGET, MODPATH, or MOD-PATH3DU.

When you are finished selecting which engine(s) to run, click 📀 (Next Step) button to proceed.

Engines Supported in the Finite Difference Numerical Workflow

The table below lists all supported engines and utilities supported in Visual MODFLOW Flex:

Flow	Transport	Utilities
 MODFLOW-2000 MODFLOW-2005 MODFLOW-NWT 	MT3DMSRT3D	 ZONEBUDGET and MODPATH MOD-PATH3DU
MODFLOW-6	MODFLOW-6	ZONEBUDGET
MODFLOW-LGR		
MODFLOW-SURFA	MODPATH	
• SEAWAT		

Notes:

- MODFLOW-LGR should only be run when you have defined a child grid.
- MODFLOW-6, MODFLOW-SURFACT, and SEAWAT are coupled flow and transport models and are incompatible with MT3DMS or RT3D.
- The MODFLOW engines can be run without any requirements from any of the other engines.
- The MODPATH engine requires a valid .BGT file to be present in the project folder. This file will be automatically created if MODFLOW and MODPATH are mutually selected.
- The Zone Budget engine requires a valid .BGT file to be present in the project folder. This file will be automatically created if MODFLOW and Zone Budget are mutually selected.
- MODFLOW-6 includes a number of significant differences when compared to other engines. If you are not familiar with MODFLOW-6 and how it has been implemented in Visual MODFLOW Flex, at a minimum, please read the the <u>Introduction to MODFLOW-6</u> as well as the discussions about translating MODFLOW-6 groundwater flow (<u>GWF</u>) and (<u>GWT</u>) models.

For more information on which flow and transport engines are compatible with the supported modeling objectives, see the respective sections on <u>Flow</u> and <u>Transport</u> modeling objectives.

Using a Previous Flow Engine Run

When running a standalone transport engine (such as MT3D-MS or RT3D) or a utility (such as MODPATH or ZoneBudget), in order to save some time, you may wish to reuse the results of a previous flow engine run, particularly if you need to rerun the configuration repeatedly. Provided you have run the flow engine at least once, you can select the "Use a previous flow engine run (if available)" option. If this option is selected and you proceed to the <u>Translation</u> step, the flow engine settings will be hidden, since the previous flow engine settings will be reused.

10.10 Translation Settings

The translate step allows you to translate the model into the input files that the applicable engine(s) will run. There are also settings for each engine that allow you to make

adjustments to how the model is run (e.g. solver settings, alternative initial heads, output control, and individual package settings).

The translation step consists of two vertical panels. The left panel includes a tree structure that lists the engine(s) selected at the <u>Select Engines</u> step and associated settings for each applicable engine. The panel on the right displays the settings (and controls) for the selected node on the translation tree. Each sub-topic in this section of the documentation describes the available settings for each node on the translation tree.

🕒 🕑 🕨 Translate												
Define Modeling Objectives	🕲 i 🗖 @ Ø											
Define Boundary Conditions	Settings Translation Log nam	TDIS	IMS	DIS	IC	OC	NPF	CHD	CHD(2)	RIV	WEL	nam(2)
 Select the Next Step Define Concervations Define Conce Budget Zones Define Conce Budget Zones Define Concervations Define Concervati	General General Settings Solvers Settings Solvers Solvers Recharge and EVT Lake Rewetting Initial Heads Arisotropy Output Control Advanced Settings	Q	Gener Output Start D.	Folder					C:\Use 1/1/20		L	enta \ Misual MODFLOW Rex\Tutorials\Conceptual M

Tools

The following tools and buttons are available at the translation step:

- **P**Translate Translate: initiates model translation
- **Open**: opens a file dialog in the folder path of the current run so that you can select and open a model input file.
- **Tabs**: toggles the layout of the translated tabs tabs can be displayed along a single line with scrolling arrows (default) or along multiple lines.
- G Previous/Next Error: jumps to the previous/next error or warning in the translation log.

Upon translation of your model, Visual MODFLOW Flex will open a new tab that displays the translation log, and convert input data for the current run in the workflow in the model explorer to that input data files required for the selected numeric engines (see <u>Appendix A</u> for details) - one tab is added to for each model package in the run. You can click any of these packages to view the contents of the corresponding input file. You can also edit these and save your changes by right-clicking in the package window and selecting save or by

typing CTRL S. Note that your changes will be overwritten if you re-translate your model and the package advanced setting for translation is set to "Yes".

General Settings

At the General Settings page you can see the following information:

- Output Directory: the folder path where the translated engine files are stored.
- Model Start Date: the start date will be the same as that which you specified in the Define Modeling Objectives step.

Engine/Package Translation Settings

This chapter covers the following topics:

- MODFLOW Translation Settings:
 - o <u>General</u>
 - o <u>Solvers</u>
 - o Recharge and Evapotranspiration
 - o Layer Types
 - o Cell Rewetting
 - o Initial Heads
 - o Anisotropy
 - o Output Control
 - o Advanced Settings

MODFLOW-6 Translation Settings*:

- o <u>General</u>
- o MODFLOW-6 Settings
- o Solver Settings
- o Initial Heads
- o Output Control
- o Advanced Settings

MODFLOW-6 Transport Translation Settings*:

- o General Settings
- o Solver Settings
- o Initial Concentrations
- o Output Control
- o Advanced Settings
- * Note: MODFLOW-6 includes a number of significant differences when compared to other engines. If you are not familiar with MODFLOW-6 and how it has been implemented in Visual MODFLOW Flex, at a minimum, please read <u>Introduction to</u> <u>MODFLOW-6</u> and the settings listed above.

MODPATH Translation Settings

- MOD-PATH3DU Translation Settings
- MT3DMS Translation Settings
 - o <u>General</u>
 - o Solution Method
 - o Output Control

SEAWAT Translation Settings

- o Dispersion (DSP) Package Settings
- o Variable Density Flow (VDF) Package Settings
- o Viscosity (VSC) Package Settings

10.10.1 MODFLOW

This chapter describes the features, functionality, and options in the Translation section of the Visual MODFLOW Flex interface. The Translation section is where the MODFLOW packages are generated.

Depending on the numeric engine selected for running the flow simulation, the MODFLOW tree item may appear as MODFLOW-2000, MODFLOW-2005, MODFLOW-NWT, MODFLOW-LGR, MODFLOW-SURFACT, or SEAWAT. Note that the settings for MODFLOW-6 are significantly different from other versions of MODFLOW and are described in a separate MODFLOW-6 section.

Please Note: SEAWAT is a coupled variable-density flow and transport model that is based on linking modified versions of the MODFLOW-2000 and MT3DMS engines. As such, the translation settings related to transport for MODFLOW-2000 also apply to SEAWAT.

For more information on the SEAWAT-specific packages see the <u>SEAWAT</u> section.

This section covers the following topics:

- General
- Solvers
- <u>Recharge and Evapotranspiration</u>
- Layer Types
- <u>Cell Rewetting</u>
- Initial Heads
- Anisotropy
- <u>Output Control</u>
- Advanced Settings

10.10.1.1 General

If this node of the translation tree is selected, Visual MODFLOW Flex will display the following (read-only) information about the model simulation:

- **Output folder**: where the translated files will be generated.
- Start date: the start date will be the same as that which you specified in the <u>Define</u> <u>Modeling Objectives</u> step

🕒 🕑 🕨 Translate													
Define Modeling Objectives	🍳 🗇	6.0											
Define Boundary Conditions	Settings	Translation Log nam	TDIS	IMS	DIS	IC	OC	NPF	CHD	CHD(2)	RIV	WEL	nam(2)
- Select the Next Step	Gene		~	Genera	al								
		Settings		Output I								\Docume	ents\Visual MODFLOW Flex\Tutorials\Conceptual M
Maget Zones		FLOW-2005		Start Da	te					1/1/200	00		
Define Particles		Settings											
PEST Run		Solvers Recharge and EVT											
Single Run		ake											
Translate		ayers											
Run Numerical Engines		Rewetting											
🖕 📥 View Results		nitial Heads											
View Charts		Anisotropy											
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10.10.1.2 MODFLOW Settings

The following settings are available for the active MODFLOW engine:

Property Package: options are available according to which flow engine is active. For:

- MODFLOW-2000, MODFLOW-2005, MODFLOW-LGR: the layer-property flow (LPF), block-centered flow (BCF), or hydrogeologic-unit flow (HUF) packages may be used
- **MODFLOW-NWT**: the upstream weighting (UPW) package must be used, and for
- MODFLOW-SURFACT: the block-centered flow package (BCF4) must be used.

Run Type: Steady-State or Transient

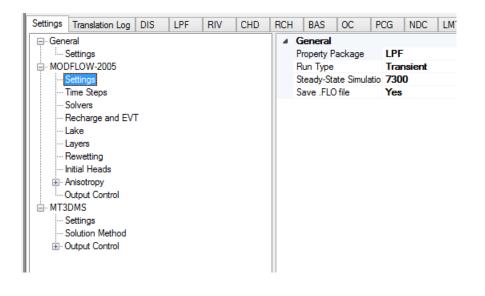
If the Steady-State Flow option is selected, Visual MODFLOW Flex will prepare the data set for a steady-state flow simulation, and will automatically use the data from the first time period (only) of each boundary condition and pumping well defined in Visual MODFLOW Flex to run the model to achieve flow equilibrium (i.e. a time-independent solution since all inputs are constant).

Please Note: if running a steady-state model, at least one boundary condition with a head of known elevation must be specified (e.g. constant head, river stage, drain bottom, or general head elevation).

If the Transient Flow option is selected, Visual MODFLOW Flex will prepare the data set for a transient flow simulation. During this process, Visual MODFLOW Flex will automatically merge all of the different time period data defined for each pumping well and boundary condition into the stress period format required by the different versions of MODFLOW. This creates a time-dependent flow solution, as the model is being run with different inputs at different times.

Steady-State Simulation Time: specified time for the mass balance terms in a steady-state run.

Save the .FLO file: toggle to save the .FLO file which can be used for MODPATH and transport (MT3DMS/RT3D) runs.



Stress Periods and Time Steps

The Time Steps option is only available when you are running a transient model (i.e. when Transient Flow run type is selected). For transient flow simulations, Visual MODFLOW Flex will automatically merge all of the different time periods defined for all of the different pumping wells and boundary conditions into the uniform stress period format required by MODFLOW. A stress period is defined as a time period in which all the stresses (boundary conditions, pumping rates, etc.) on the system are constant. Unfortunately, the data collected for each modeling site is rarely synchronized in terms of stress periods, so Visual MODFLOW Flex merges the time schedules for all pumping wells and boundary conditions to determine the length of each stress period for a transient simulation. As a result, the user cannot directly modify the number of stress periods or the length of each stress period.

The Time step options window (as shown in the following figure) is used to define the number of Time steps in each stress period and the time step Multiplier is used to increment each time step size.

Settings Translation Log											
General	✓ General										
Settings	Property Pack	age		LPF							
MODFLOW-2005	Run Type			Transient							
Settings	Steady-State	Simulation Time		1							
Solvers	Save .FLO file	;		No							
···· Recharge and EVT											
Lake											
Layers											
Rewetting											
Initial Heads											
Anisotropy											
Output Control											
Advanced Settings	Run Type										
E RT3D250	Simulation Type: S	Steady-State or Tra	insient								
General Solution Method											
Output Control											
	Time Steps Val	ue									
	Stress Period	Start	End	Time Steps	Multiplier	Steady-State					
	1	0	7300	10	1.2						

The Stress Period column indicates the stress period number while the Start and End columns indicate the start time and end time, respectively, for each stress period.

Each stress period is divided into a user-defined number of Time steps whereby the model will calculate the head solution at each time step. The default value for Time steps is 10.

The time step Multiplier is the factor used to increment the time step size within each stress period (i.e. it is the ratio of the value of each time step to that of the preceding time step). The default value is 1.2. A time step Multiplier value greater than 1 will produce smaller time steps at the beginning of a stress period resulting in a better representation of the changes of the transient flow field. Thus increasing the number of time steps in a simulation may result in smoother head or drawdown versus time curves.

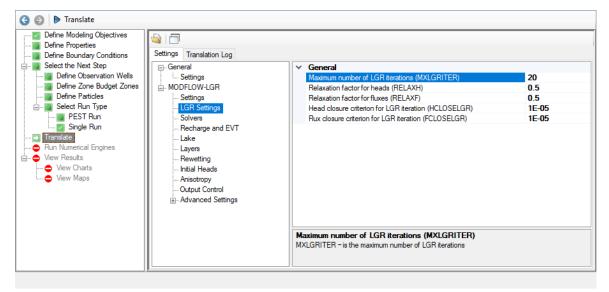
The steady-state column indicates if the stress period is transient or steady-state. This option is available if MODFLOW-2000, MODFLOW-2005, or MODFLOW-SURFACT is selected as the numeric engine for the flow model. These engines allow individual stress periods in a single simulation to be either transient or steady state instead of requiring the entire simulation to be either steady state or transient. Steady-state and transient stress periods can occur in any order. Commonly the first stress period may be run as steady state, to produce a solution that is used as the initial condition for subsequent transient stress periods.

Accommodating Boundary Conditions with Varying End Times

Visual MODFLOW Flex allows you to define boundary conditions with varying end times; the number of stress periods for the model will be calculated from the end time of the longest boundary condition. If there is a stress period where there are no data defined for a boundary condition, then you will see an entry of "0" in the appropriate package, for that

stress period; this denotes that zero cells are defined for that stress period. In the case of pumping wells, you will see a rate of 0 for the well cells.

10.10.1.3 LGR settings



The Local Grid Refinement (LGR) package, which is only available for MODFLOW-LGR simulations:

- 1. Identifies the parent and child grids,
- 2. Specifies how they related to one another, and
- 3. Controls the coupling iterations between them.

Visual MODFLOW Flex automatically handles the first two items, while the coupling between the parent and child models are defined using the following settings:

- MXLGRITER: the maximum number of LGR iterations, a positive integer value
- RELAXH: relaxation factor for heads, values must be between 0 and 1
- RELAXF: relaxation factor for fluxes, values must be between 0 and 1
- HCLOSELGR: head closure criterion for LGR coupling iterations
- FCLOSELGR: flux closure criterion for LGR coupling iterations

For mode information please refer to the MODFLOW-LGR Documentation by Mehl and Hill (2013) or the USGS <u>Online Guide</u>.

10.10.1.4 Solvers

Visual MODFLOW Flex comes with a choice of different solvers to use in solving the numerical equations for the flow simulation:

🔄 🗂 🍇 Update Solver		
Settings Translation Log DIS	UPW RIV CHD RCH FHB BAS	OC GAG NWT NDC LMT IN E
🖃 - General	✓ General	
Settings	Selected Solver	Conjugate Gradient Solver (PCG)
MODFLOW-2005		
···· Settings	 PCG2 Settings 	
Solvers	Max. outer iteration (MXITER)	100
···· Recharge and EVT	Max. inner iteration (ITER1)	25
Lake	Pre-conditioning method (NPCOND)	Modified Incomplete Cholesky (NPCOND=1)
Layers	Head change criterion (HCLOSE)	1E-05
···· Rewetting	Residual criterion (RCLOSE)	0.0001
···· Initial Heads	Relaxation parameter (RELAX)	1
Anisotropy	Estimate of the upper bound (NBPOL)	Calculate esimate
Output Control	The printout interval (IPRPCG)	10
Advanced Settings	Convergence output control (MUTPCG)	Print only the number of iterations(MUTPCG=1)
i⊟ MT3DMS	Damping factor (DAMP/DUMPPCG)	1
General	Damping factor for transient stress period (DUN	MP 1
Solution Method		
Output Control		
ia. Advanced Settings □. MODPATH		
Discharge Options		
Discharge Options	Max. outer iteration (MXITER)	
	Max. outer iteration	

- Preconditioned Conjugate-Gradient Package (PCG2)
- <u>Strongly Implicit Procedure Package (SIP)</u>
- <u>Slice-Successive Overrelaxation Package (SOR)</u>
- WHS Solver for VMOD Flex (WHS)
- Geometric Multigrid Solver (GMG)
- Systems Algebraic Multi-Grid Solver (SAMG) (see below)
- <u>Newton-Raphson Solver (NWT)</u> only available with MODFLOW-NWT

These solvers and their individual settings can be accessed by selecting MODFLOW/Solver from the Run section of Visual MODFLOW Flex. A Solver Setting window will appear, similar to the image shown in the following figure, with a list for choosing the desired Solver and a listing of the settings for the selected Solver.

Please Note: the SAMG solver is available in the editions of Visual MODFLOW Flex as follows:

- Basic Edition: not available
- Professional Edition: SAMG single core only
- Premium Edition: SAMG multi-core/parallel processing

Update Solvers

The update solver [Update Solver] button allows you to update/translate the solver package settings, since it is common to adjust only the solver settings when (re)-running a

model. This allows you to quickly readjust the values more efficiently than translating the whole model.

10.10.1.4.1 PCG

The PCG solver (PCG2, in MODFLOW-SURFACT) uses the preconditioned conjugategradient method to solve the simultaneous equations produced by the model. Linear and non-linear flow conditions may be simulated. PCG includes two preconditioning options: modified incomplete Cholesky preconditioning, which is efficient on scalar computers; and polynomial preconditioning, which requires less computer storage and, with computer specific modifications, is most efficient on vector computers. Convergence of the solver is determined using both the head-change and residual criteria. Non-linear problems are solved using the Picard iterations. The PCG Package is described in USGS Water-Resources Investigations Report 90-4048 (Hill, <u>1997</u>).

The PCG solver works on a two-tier approach to a solution at one time step, inner and the outer iterations. Outer iterations are used to vary the pre-conditioned parameter matrix in an approach toward the solution. An outer iteration is where the hydrogeologic parameters of the flow system are updated (i.e., transmissivity, saturated thickness, storativity) in the preconditioned set of matrices. The inner iterations continue until the user-defined maximum number of inner iterations are executed, or the final convergence criteria are met. The outer iterations continue until the final convergence criteria are met on the first inner iteration after an update.

The following is a description of the solver parameters for the PCG method:

- Maximum Number of Outer Iterations: [Default = 25] This parameter provides an upper limit on the number of outer iterations to be performed. The maximum number of iterations will only be used if a convergent solution is not reached beforehand. Twenty-five iterations should be adequate for most problems. However, if the maximum number of outer iterations is reached and an appropriate mass balance error is not achieved, this value should be increased.
- Maximum Number of Inner Iterations: [Default = 10] This parameter provides an upper limit on the number of inner iterations to be performed. This number of iterations will only be used if a convergent solution for the current set of matrices in the "outer" iteration is not reached beforehand. Ten inner iterations should be adequate for most problems. More than ten iterations will not usually improve the solution, as the solution is updated again when it returns to the outer iterations.
- Head Change Criterion for Convergence: [Default = 0.01] After each outer iteration has completed, the solver checks for the maximum change in the solution at every cell. If the maximum change in the solution is below a set convergence tolerance (set here in the working units feet or meters) then the solution has converged and the solver stops, otherwise a new outer iteration starts.
- A solution accurate to 0.01 [ft. or m] will normally be sufficient for most problems, unless the maximum head difference across the modeled domain is less than one foot or meter. If an appropriate mass balance is not achieved and the number of inner and outer iterations are within the maximums declared above, this value can be decreased by an order of magnitude, e.g. 0.001.

 Residual Criterion for Convergence: [Default = 0.01] While the head change criterion is used to judge the overall solver convergence, the residual criterion is used to judge the convergence of the inner iterations of the solver. If the maximum absolute value of the residual at all nodes is less than the tolerance specified here (units of L³/T) then the solver will proceed to the next outer iteration.

If you notice that only a few inner iterations are being performed for all outer iterations, and an appropriate mass balance is not achieved, the Residual Criterion value can be decreased by one or more orders of magnitude.

Note: The residual criterion is unit-dependent. The default value of 0.01 is often sufficient if your length units are feet or meters and your time units are seconds. If your time units are not seconds, you should multiply the default value by the number of seconds in your time unit (e.g. use a residual criterion of 0.01 * 86400, if your time unit is days).

- Damping Factor: [Default = 1] This factor allows the user to reduce (dampen) the head change calculated during each successive outer iteration. For most "well posed" and physically realistic groundwater flow problems, the damping factor of one will be appropriate. This parameter can be used to make a non-convergent (oscillating or divergent) solution process more stable such that a solution will be achieved. This is done by decreasing the damping factor to a value between 0 and 1 (only rarely < 0.6). This parameter is similar to the "acceleration parameters" used in other solvers.
- Printout Interval: [Default =10] The printout interval is the number of iterations after which the maximum head change (and residual) of the solution is written to the listing (.LST) file.
- If the Preconditioning Method is set to Cholesky, the Relaxation parameter can be set. Although the default is 1, in some cases a value of 0.97-0.99 may reduce the number of iterations required for convergence.

10.10.1.4.2 GMG

The GMG solver, based on the preconditioned conjugate gradient algorithm, has been developed by the USGS for solving finite-difference based flow models. As opposed to AMG, the preconditioning in GMG is based on a solver method known as geometric multigrid. The GMG solver has been demonstrated to greatly reduce model run times relative to other solvers using a comparable amount of memory. Detailed information about the GMG solver, including comparisons with the AMG solver, can be found in the GMG Linear Equation Solver Package PDF documentation.

The solver parameters for the Geometric Multigrid Solver are described below using excerpts from the GMG Linear Equation Solver Package PDF documentation:

- Max. outer iterations (MXITER): The maximum number of outer iterations. For linear problems, MXITER can be set to 1. For nonlinear problems, MXITER needs to be larger, but rarely more than 100. The maximum number of iterations will only be used if a convergent solution is not reached beforehand.
- Max. inner iterations (IITER): The maximum number of PCG iterations for each linear solution. A value of 100 is typically sufficient. It is frequently useful to specify a smaller

number for nonlinear problems so as to prevent an excessive number of inner iterations. This number of iterations will only be used if a convergent solution for the current set of matrices in the "outer" iteration is not reached beforehand.

- Adaptive Damping Control (IADAMP): IADAMP is a flag that controls adaptive damping. If IADAMP = 0, then the value assigned to DAMP is used as a constant damping parameter. If IADAMP ≠ 0, then the value of DAMP is used for the first nonlinear iteration. The damping parameter is adaptively varied on the basis of the head change, using Cooley's method for subsequent iterations.
- Head change criterion (HCLOSE): After every outer iteration is completed, the solver checks for the maximum change in the solution at every cell. If the maximum change in the solution is below a set convergence tolerance (set here in the working units of feet or metres) then the solution has converged and the solver stops, otherwise a new outer iteration is started. A solution accurate to 0.01 [ft. or m] will normally be sufficient for most problems unless the maximum head change throughout the modeled domain is less than 1 foot or metre. If an appropriate mass balance is not achieved and the number of inner and outer iterations is within the maximums, this value can be decreased by an order of magnitude.
- Residual criterion (RCLOSE): RCLOSE is the residual convergence criterion for the inner iteration. The PCG algorithm computes the l2-norm of the residual and compares it against RCLOSE Typically, RCLOSE is set to the same value as HCLOSE (see below). If RCLOSE is set too high, then additional outer iterations may be required due to the linear equation not being solved with sufficient accuracy. On the other hand, a too restrictive setting for RCLOSE for nonlinear problems may force an unnecessarily accurate linear solution. This may be alleviated with the IITER parameter or with damping.
- Relaxation parameter (RELAX): The RELAX parameter can be used to improve the spectral condition number of the ILU preconditioned system. The value of RELAX should be approximately one. However, the relaxation parameter can cause the factorization to break down. If this happens, then the GMG solver will report an assembly error and a value smaller than one for RELAX should be tried. This item is read only if ISC = 4.
- Upper bound of estimate (NPBOL): IOUTGMG is a flag that controls the output of the GMG solver. The possible values of IOUTGMG and their meanings are as follows: If IOUTGMG = 0, then only the solver inputs are printed. If IOUTGMG = 1, then for each linear solve, the number of PCG iterations, the value of the damping parameter, the I2-norm of the residual, and the max-norm of the head change and its location (column, row, layer) are printed. At the end of a time/stress period, the total number of GMG calls, PCG iterations, and a running total of PCG iterations for all time/stress periods are printed. If IOUTGMG = 2, then the convergence history of the PCG iteration is printed, showing the I2-norm of the residual and the convergence factor for each iteration. IOUTGMG = 3 is the same as IOUTGMG = 1 except output is sent to the terminal instead of the MF2K LIST output file. IOUTGMG = 4 is the same as IOUTGMG = 2 except output is sent to the terminal instead of the MF2K LIST output file.
- Multigrid Preconditioner (ISM): ISM is a flag that controls the type of smoother used in the multigrid preconditioner. The possible values for ISM and their meanings are as follows: If ISM = 0, then ILU(0) smoothing is implemented in the multigrid preconditioner. This smoothing requires an additional vector on each multigrid level to store the pivots in the ILU factorization. If ISM = 1, then Symmetric Gauss Seidel (SGS) smoothing is implemented in the multigrid preconditioner. No additional storage is required for this smoother; users may want to use this option if available memory is

exceeded or nearly exceeded when using ISM = 0. Using SGS smoothing is not as robust as ILU smoothing; additional iterations are likely to be required in reducing the residuals. In extreme cases, the solver may fail to converge as the residuals cannot be reduced sufficiently.

- Semicoarsening Control in the Multigrid Preconditioner (ISC): A flag that controls semicoarsening in the multigrid preconditioner. The possible values of ISC and their meanings are given as follows: If ISC = 0, then the rows, columns and layers are all coarsened. If ISC = 1, then the rows and columns are coarsened, but the layers are not. If ISC = 2, then the columns and layers are coarsened, but the rows are not. If ISC = 3, then the rows and layers are coarsened, but the columns are not. If ISC = 4, then there is no coarsening. Typically, the value of ISC should be 0 or 1. In the case that there are large vertical variations in the hydraulic conductivities, then a value of 1 should be used. If no coarsening is implemented (ISC = 4), then the GMG solver is comparable to the PCG2 ILU(0) solver described in Hill (1990) and uses the least amount of memory.
- Damping factor (DAMP): This factor allows the user to reduce (dampen) the head change calculated during each successive outer iteration. For most "well posed" and physically realistic groundwater flow problems, the dampening factor of one will be appropriate. This parameter can be used to make a non-convergent (oscillating or divergent) solution process more stable such that a solution will be achieved. This is done by decreasing the damping factor to a value between 0 and 1 (only rarely < 0.6). This parameter is similar to "acceleration parameters" used in other solvers

10.10.1.4.3 WHS

The WHS Solver uses a Bi-Conjugate Gradient Stabilized (Bi-CGSTAB) acceleration routine implemented with Stone incomplete decomposition for preconditioning of the groundwater flow partial differential equations. This solver, as all iterative solvers, approaches the solution of a large set of partial differential equations iteratively through an approximate solution. Because the matrix equation for groundwater flow is initially "ill-conditioned", effective preconditioning of these matrices is necessary for an efficient solution.

The WHS solver works on a two-tier approach to a solution at one time step. Outer iterations are used to vary the factorized parameter matrix in an approach toward the solution. An outer iteration is where the hydrogeologic parameters of the flow system are updated (i.e., transmissivity, saturated thickness, storativity) in the factorized set of matrices. Different levels of factorization allow these matrices to be initialized differently to increase the efficiency of solution and model stability. Inner iterations are used to iteratively solve the matrices created in the outer iterations.

The solver parameters for the WHS method are described below:

- Maximum Number of Outer (non-linear) Iterations: [Default = 50] This parameter
 provides an upper limit on the number of outer iterations to be performed. The
 maximum number of iterations will only be used if a convergent solution is not reached
 beforehand. Fifty iterations should be adequate for most problems. However, if the
 maximum number of outer iterations is reached and an appropriate mass balance error
 is not achieved, this value should be increased.
- Maximum Number of Inner Iterations: [Default = 25] This parameter provides an upper limit on the number of inner iterations to be performed. This number of iterations will only be used if a convergent solution for the current set of matrices in the "outer"

iteration is not reached beforehand. Twenty-five inner iterations should be adequate for most problems. However, if the maximum number of inner iterations was used for all outer iterations and an appropriate mass balance error was not achieved, this value can be increased.

- Head Change Criterion for Convergence: [Default = 0.01] After every outer iteration is completed, the solver checks for the maximum change in the solution at every cell. If the maximum change in the solution is below a set convergence tolerance (set here in the working units of feet or metres) then the solution has converged and the solver stops, otherwise a new outer iteration is started. A solution accurate to 0.01 [ft. or m] will normally be sufficient for most problems unless the maximum head change throughout the modeled domain is less than 1 foot or metre. If an appropriate mass balance is not achieved and the number of inner and outer iterations is within the maximums, this value can be decreased by an order of magnitude.
- Residual Criterion for Convergence: [Default = 0.01] While the head change criterion is used to judge the overall solver convergence, the residual criterion is used to judge the convergence of the inner iterations of the solver. If the change in successive inner iterations is less than the tolerance specified here (in working units of feet or metres), then the solver will proceed with the next outer iteration. The residual criterion for convergence of 0.001 should be appropriate for most problems. However, if you notice that only a few inner iterations are being performed for every outer iteration and an appropriate mass balance is not achieved, this parameter value can be decreased by one or more orders of magnitude.
- Damping Factor for the Outer Iterations: [Default = 1] This factor allows the user to reduce (dampen) the head change calculated during each successive outer iteration. For most "well posed" and physically realistic groundwater flow problems, the dampening factor of one will be appropriate. This parameter can be used to make a non-convergent (oscillating or divergent) solution process more stable such that a solution will be achieved. This is done by decreasing the damping factor to a value between 0 and 1 (only rarely < 0.6). This parameter is similar to "acceleration parameters" used in other solvers.
- Relative Residual Criterion: [Default = 0] This parameter provides another method of checking for convergence of the inner iteration. This method compares the residual from the most recent inner iteration to the residual from the initial inner iteration. Once the most recent inner iteration residual is below the initial inner iteration residual times the relative residual criterion, the current outer iteration is completed and a new outer iteration will be started.
- Factorization Level: [Default = 0] There are two "levels" of factorization available with the WHS solver, 0 and 1. Level 0 requires more outer iterations but less memory. Level 1 requires fewer outer iterations but more memory. While convergence of the solver requires fewer iterations with a factorization level of 1, the memory required to run the solver increases with this factorization level. Also, the work per iteration increases with the level 1 factorization such that the total solution time may not be less than the solution time using level 0 factorization.

10.10.1.4.4 SIP

The Strongly Implicit Procedure, also known as SIP, is a method for solving a large system of simultaneous linear equations by iterations. The advantage of the SIP solver is that it is very stable and generally converges to a solution, but often very slowly. It is not as fast as the PCG method, but it requires less memory to compute the final solution. Because each equation involves up to seven unknown values of head, and because the set of unknown

values changes from one equation to the next throughout the grid, the equations for the entire grid must be solved simultaneously at each time step. This package is described in Chapter 12 of the MODFLOW manual included with your Visual MODFLOW Flex media, in the Manual folder.

The solver parameters for the SIP method are described below:

- Maximum Number of Iterations: [Default = 200] This is the upper limit on the number of iterations to be performed. The maximum number of iterations will only be considered if a convergent solution is not reached beforehand. Two hundred iterations should be adequate for most problems. However, if the maximum number of iterations is reached and an appropriate mass balance error is not achieved, this value should be increased.
- Number of Iteration Parameters: [Default = 5] The finite difference equations describing the groundwater flow system can be put into matrix form as [A] {h}={q}. Where [A] is the coefficient matrix, {h} is the heads array and {q} is the flux array. The number of iteration parameters indicates the number of parameters that will be used to transform the initial coefficient matrix [A] to a similar matrix that can be decomposed into two lower and upper triangular matrices [L] and [U], respectively. The default value of 5 is generally sufficient.
- Acceleration Factor: [Default = 1] The acceleration factor controls the magnitude of head change between iterations. The acceleration factor must be positive. Values larger than one will result in larger head changes between iterations; the solution may be approached faster but it may also overshoot the solution more easily. Values less than one will result in smaller head changes, requiring more iterations to reach a solution.
- Head Change Criterion for Convergence: [Default = 0.01] After each iteration is completed, the solver checks for the maximum change in the solution at every cell. If the maximum change in the solution is below a set convergence tolerance (set here in the working units of feet or metres) then the solution has converged and the solver stops, otherwise a new iteration is started. A solution accurate to 0.01 [ft. or m] will normally be sufficient for most problems unless the maximum head change throughout the modeled domain is smaller than one foot or metre. If an appropriate mass balance is not achieved and the maximum number of iterations is not reached, this value can be decreased by an order of magnitude.
- Printout Interval: [Default =10] The printout interval is the number of iterations after which the maximum head change (and residual) of the solution is written to the listing (.LST) file.
- User Seed Value: [Default = 0.01] There are two options: either the user can enter the seed, or the seed will be calculated at the start of the simulation from problem parameters. The iteration parameter 'seed' is used as a basis for determining the sequence of w values. The w multiplies each term on the right side of the equation; and must be cycled through a series of values in successive iterations to achieve satisfactory rates of convergence. The more strongly diagonal the coefficient matrix, the less important the choice of seed will be.

10.10.1.4.5 SOR

Slice-Successive Over-Relaxation is a method for solving large systems of linear equations iteratively. It is implemented in the SOR Package by dividing the finite difference grid into vertical slices, and grouping the node equations into discrete sets, each set corresponding to a slice. In every iteration, these sets of equations are processed in turn, resulting in a new set of estimated head values for each slice. As the equations for each slice are processed,

they are first expressed in terms of the changes in computed heads between successive iterations. The set of equations corresponding to the slice is then solved directly by Gaussian elimination, treating the terms for adjacent slices as known quantities. The values of head change computed for the slice are then each multiplied by an acceleration variable, T. The results are taken as the final values of head change in that iteration for the slice. This procedure is repeated for each slice in sequence until all of the slices in the three-dimensional array have been processed, thus completing a domain iteration. The entire sequence is then repeated, until the differences between the head values computed in successive iterations are less than the chosen criterion at all nodes in the mesh. The SOR Package is described in detail in Chapter 13 of the MODFLOW reference manual included with your VMOD Flex media, in the Manual folder.

The solver parameters for the SOR method are described below:

- Maximum Number of Iterations: [Default = 50] This parameter provides an upper limit on the number of iterations to be performed. The maximum number of iterations will only be used if a convergent solution is not reached beforehand. 50 iterations should be adequate for most problems. However, if the maximum number of outer iterations is reached and an appropriate mass balance error is not achieved, this value should be increased.
- Acceleration Factor: [Default = 1] The acceleration factor controls the magnitude of head changes between iterations. The acceleration factor must be positive. Values larger than one will result in larger head changes between iterations; the solution may be approached faster but it may also overshoot the solution more easily. Values less than one will result in smaller head changes, thus, requiring more iterations to reach a solution.
- Head Change Criterion for Convergence: [Default = 0.01] After each iteration is completed, the solver checks for the maximum change in the solution at every cell. If the maximum change in the solution is below a set convergence tolerance (set here in the working units of feet or metres), then the solution has converged and the solver stops, otherwise a new iteration is started. A solution accurate to 0.01 [ft. or m] will normally be sufficient for most problems unless the maximum head change throughout the model domain is less than 1 foot or metre. If an appropriate mass balance is not achieved and the number of iterations is less than the maximum, this value can be decreased by an order of magnitude.
- Printout Interval: [Default =10] The printout interval is the number of iterations after which the maximum head change (and residual) of the solution is written to the listing (.LST) file.

10.10.1.4.6 SAMG

Visual MODFLOW Flex supports the Algebraic Multigrid Methods for Systems Solver (SAMG) Package developed by the Fraunhofer Institute for Algorithms and Scientific Computing (FhG-SCAI).

Please Note: the SAMG solver is only compatible with the MODFLOW-2000, -2005, -LGR, and -USG flow engines. The SAMG solver is available in single-core mode in Visual MODFLOW PRO and in multi-core mode in Visual MODFLOW Premium. The Algebraic Multigrid (AMG) Package solver may be obtained from the Fraunhofer Institute for Algorithms and Scientific Computing (FhG-SCAI) for research purposes only.

The SAMG solver package is a complete multi-level framework, designed to overcome the high memory requirements of previous AMG-based solvers, while maintaining the scalability and rapid execution times. Testing of the SAMG solver vs. the PCG2 solver using several models generated using Visual MODFLOW demonstrated solution times to be faster by a factor of between 2.4 and 11.3. The SAMG Package has some distinct advantages over other solvers available with MODFLOW for problems with large grids (more than about 40,000 cells) and/or a highly variable hydraulic-conductivity field. The advantages of multigrid methods over the other iterative solvers mentioned are (1) the effectiveness of the multigrid solver is not dependent on the initial head distribution, and (2) for many problems of interest, the rate of convergence scales approximately linearly with the size of the domain, unlike the other solvers where the rate of convergence increases nonlinearly (<u>Demmel, 1997</u>).

The Solver settings window contains a number of user-defined solver settings which can influence the speed and effectiveness of the AMG solver.

- Max. Iterations (MXITER): [Default = 50] MXITER is the maximum number of times that the AMG routines will be called to obtain a solution. MXITER is never less than 2, and rarely more than 50. MXITER often equals 2 when the problem is linear (all layers are confined, and no boundary conditions are nonlinear; the Evapotranspiration, Drain, and River Packages, for example, produce nonlinear boundary conditions). For nonlinear problems, MXITER generally is 50 or less; however values near 50 and sometimes even larger are needed for more severely nonlinear problems.
- Max. Cycles (MXCYC): [Default = 50] For each call to the solver, AMG cycles through one or more sequences of coarsening and refinement. The solver is limited to a maximum of MXCYC cycles per call to the solver. For most problems, convergence for each iteration is achieved in less than 50 cycles, so that generally MXCYC can be less than 50. For highly nonlinear problems, however, better performance may be achieved by limiting the solver to a small number of cycles, and increasing the maximum number of iterations (MXITER). This prevents the solver from needlessly finding very accurate solutions at early iterations of these highly nonlinear problems.
- Residual Convergence Criterion (RCLOSE) for the inner iteration. Typically RCLOSE
 is set to the same value as HCLOSE. If RCLOSE is set too high, then additional outer
 iterations may be required due to the linear equation not being solved with sufficient
 accuracy. Likewise, a too restrictive setting for RCLOSE for nonlinear problems may
 force an unnecessarily accurate linear solution. This may be alleviated with the
 MXCYC parameter or with damping.
- Note: In the new SAMG package, RCLOSE and HCLOSE replace BCLOSE
- Damping Factor (DAMP): [Default = 1] The damping factor can be used to restrict the head change from one iteration to the next, which commonly is useful in very nonlinear problems. DAMP makes the solution change slowly, thus avoiding spurious deviations prompted by nonlinear effects at intermediate solutions. Values of DAMP less than 1.0 restrict the head change (under-relaxation), while values greater than 1.0 accelerate the head change (over-relaxation). For linear problems, no damping is necessary, and DAMP should be set equal to 1.0. For non-linear problems, restricting the head change (DAMP < 1.0) may be necessary to achieve convergence, and values of DAMP between 0.5 and 1.0 are generally sufficient.

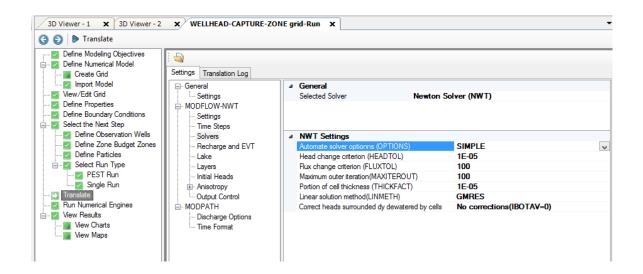
For some nonlinear problems, imposing a fixed value of DAMP for every iteration can hinder convergence. One remedy for this condition is to adjust the amount of damping depending on how the head solution progresses. The AMG Package provides two adaptive damping strategies; (1) Cooley's method with Huyakorn's modification, and (2) the relative reduced residual method. These methods are described in detail in the U.S. Geological Open-File Report 01-177. A DAMP value of -1 will utilize the first method, and a DAMP value of -2 will utilize the second method.

- Max. Damping Factor (DUP): [Default = 1] The upper limit for DAMP when an adaptive damping strategy is used.
- Min. Damping Factor (DLOW): [Default = 0.2] The lower limit for DAMP when an adaptive damping strategy is used
- Head Change Convergence Criterion (HCLOSE), similar as described for previous solvers
- Perform Conjugate Gradient Iterations (ICG): [Default = checked] In some cases, AMG can perform poorly as a result of a small number of error components that are not reduced during the AMG cycling. A few iterations of a conjugate gradient solver can often reduce these error components and thus help convergence (Cleary and others, 2000). In these cases, the parameter ICG can be set to 1 to perform conjugate gradient iterations at the end of each multigrid cycle. Activating this option can decrease execution times for some problems, but it will also increase the amount of memory used by the solver.
- The Print Flag (IOUTAMG) frame allows you to select between various print options.
- CONTROL Parameter [Default = 2]
 - 1 reuse of the setup phase is not used
 - 2 reuse of the setup phase will be used (Recommended)
 - 3 reuse of the setup phase will be used, and SSC will be used

10.10.1.4.7 NWT

The NWT Solver parameters are shown in the image below. Detailed information about MODFLOW-NWT can be found: http://water.usgs.gov/ogw/modflow-nwt/

Please Note: MODFLOW-NWT includes an upstream-weighting (UPW) intercell conductance package as a replacement internal flow package to those provided by the BCF, LPF, and HUF Packages. When MODFLOW-NWT is selected as the flow engine, the UPW property package will be generated during translation and used in the model run.



Visual MODFLOW Flex provides options for the most-commonly used parameters (head change criterion, flux change criterion, number of iterations, etc.) and to choose the solver OPTIONS (Automate Solver Options). MODFLOW-NWT provides flexibility to specify the values for each of the parameters, or to choose from one of the pre-defined solver "schemes". When you select one of the pre-defined schemes, then the solver parameters are fixed and cannot be modified (all fields will be non-visible). If choose the "SPECIFIED" option, then the full set of solver parameters will be defined in the .NWT file (using defaults) and you will have the ability to change these parameters in the .NWT file after Translation. When you choose one of the pre-defined schemes (Simple, Moderate, or Complex) then you will see only an abbreviated set of parameters.

- SPECIFIED indicates that the optional solver input values listed for items 1 and 2 will be specified in the NWT input file by the user.
- SIMPLE indicates that default solver input values will be defined that work well for nearly linear models. This would be used for models that do not include nonlinear stress packages, and models that are either confined or consist of a single unconfined layer that is thick enough to contain the water table within a single layer. (See Table 2 of package documentation for the solver input values that will be used for this option.)
- MODERATE indicates that default solver input values will be defined that work well for moderately nonlinear models. This would be used for models that include nonlinear stress packages, and models that consist of one or more unconfined layers. The "MODERATE" option should be used when the "SIMPLE" option does not result in successful convergence. (See Table 2 of package documentation for the solver input values that will be used for this option.)
- COMPLEX indicates that default solver input values will be defined that work well for highly nonlinear models. This would be used for models that include nonlinear stress packages, and models that consist of one or more unconfined layers representing complex geology and surface water/groundwater interaction. The "COMPLEX" option should be used when the "MODERATE" option does not result in successful convergence. (See Table 2 of package documentation for the solver input values that will be used for this option.)

HEADTOL (units of length)—is the maximum head change between outer iterations for solution of the nonlinear problem.

FLUXTOL (units of length cubed per time)—is the maximum root-mean-squared flux difference between outer iterations for solution of the nonlinear problem.

MAXITEROUT is the maximum number of iterations to be allowed for solution of the outer (nonlinear) problem.

THICKFACT is the portion of the cell thickness (length) used for smoothly adjusting storage and conductance coefficients to zero.

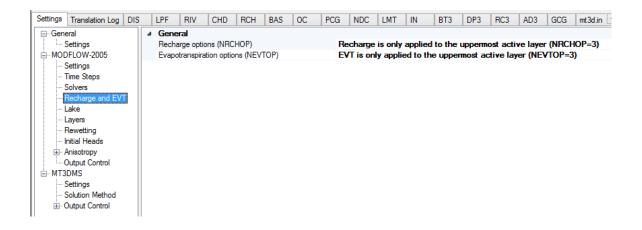
LINMETH is a flag that determines which matrix solver will be used.

- 1 = GMRES will be used
- 2 = xMD will be used

IBOTAV is a flag that indicates whether corrections will be made to groundwater head relative to the cell-bottom altitude if the cell is surrounded by dewatered cells. Checked = a correction will be made; Not-checked = no correction will be made. This input variable is problem specific and both options (IBOTAV selected/not-selected) should be tested.

Please Note: The modification to the .WEL package for variable PHIRAMP is currently not supported in Visual MODFLOW Flex

10.10.1.5 Recharge and Evapotranspiration



Recharge

The Recharge zone distribution can be applied to any of the user-specified model Layers. If the recharge is assigned to the top grid layer, and some cells in the top layer become dry during the course of the simulation, or if some cells in the top layer are designated as no-flow cells, the MODFLOW program allows the recharge to be applied to the grid cells in the upper most active (wet) layer in the model. The Recharge settings are shown in the following Recharge options window and these are described below.

- Recharge is only applied to the top grid layer: If any grid cells in Layer 1 are dry, or if they are designated as no-flow cells, the recharge values assigned to these grid cells will NOT be carried down to the underlying active (wet) grid cells. In this case, the inactive or dry cells act like an impermeable barrier to the recharge.
- Recharge is applied to the specified layer: It allows the user to assign the recharge values to any of the specified model layer
- Recharge is applied to the uppermost active layer: If any grid cells in Layer 1 are dry, or if they are designated as no-flow cells, the recharge values assigned to these grid cells will be carried down to the upper most active (wet) grid cell in the same vertical column of grid cells.

Note: A constant head boundary condition always intercepts recharge and prevents deeper infiltration.

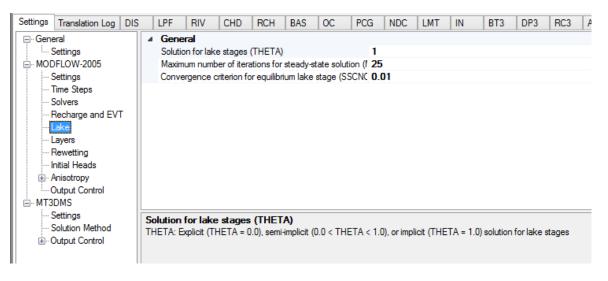
Evapotranspiration

The Evapotranspiration distribution can be applied to any of the user-specified model Layers. If assigned to the top grid layer, and some cells in the top layer become dry during the course of the simulation, or if some cells in the top layer are designated as no-flow cells, the MODFLOW program allows the Evapotranspiration to be applied to the grid cells in the upper most active (wet) layer in the model. The Evapotranspiration settings are shown in the following Evapotranspiration Options window and these are described below.

- Evapotranspiration is only applied to the top grid layer: If any grid cells in Layer 1 are dry, or if they are designated as no-flow cells, the Evapotranspiration values assigned to these grid cells will NOT be carried down to the underlying active (wet) grid cells. In this case, the inactive or dry cells act like an impermeable barrier to the Evapotranspiration.
- Evapotranspiration is applied to the specified layer: It allows the user to assign the Evapotranspiration values to any of the specified model layers.
- Evapotranspiration is applied to the uppermost active layer: If any grid cells in Layer 1 are dry, or if they are designated as no-flow cells, the evapotranspiration values assigned to these grid cells will be carried down to the upper most active (wet) grid cell in the same vertical column of grid cells.

10.10.1.6 Lakes

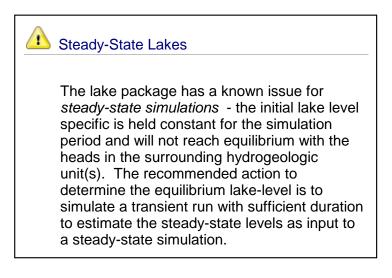
The following settings are supported in Visual MODFLOW Flex for the LAK package and facilitate the internal flow balance for the LAK package:



THETA: variable to specify an explicit (THETA=0.0), semi-implicit (0.0<THETA<1.0), or fully implicit (THETA=1.0) solution for lake stages

MSSITR: Maximum number of iterations for steady-state solution

SSCNCR: Convergence criterion for equilibrium lake stage solution by Newton's method.



10.10.1.7 Layer Types

Settings Translation Log DIS	LPF	RIV	CHD	RCH	BAS	OC	PCG	NDC	LMT	IN	BT3	DP3	RC3	AD3	GCG	mt3d.in 4	
⊡. General Settings	Layer number		LAYCON	I		Interbl	lock Tran	ismissivity			Layer Type						
MODFLOW-2005	1	:	3		00: Harmo	nic mear	n i				3: Conf	ined/Unc	onfined,	variable	5, T		
···· Settings ···· Time Steps	2	:	3		00: Hamonic mean							3: Confined/Unconfined, variable S, T					
Solvers	3	3	3		00: Harmo	nic mear	n i				3: Conf	ined/Unc	onfined,	variable	5, T		
Recharge and EVT Lake Layes Rewetting Initial Heads Anisotropy Output Control MT3DMS Solution Method Output Control Output Control																	

The Layer Type Settings window is used to set the LAYCON value and the LAYAVG variables required by the MODFLOW numeric engine.

The LAYCON value is the layer-type index array recognized by MODFLOW. MODFLOW has four different Layer Types to choose for LAYCON values as described below:

- Type 0 Confined: Transmissivity and storage coefficients of the layer are constant for the entire simulation.
- Type 1 Unconfined: Transmissivity of the layer varies and is calculated from the saturated thickness and hydraulic conductivity. The storage coefficient is constant; valid only for Layer 1.
- Type 2 Confined/Unconfined: Transmissivity of the layer is constant. The storage coefficient may alternate between confined and unconfined values.
- Type 3 Confined/Unconfined: [Default setting] Transmissivity of the layer varies. It is calculated from the saturated thickness and hydraulic conductivity. The storage coefficient may alternate between confined and unconfined values. Vertical leakage from above is limited if the aquifer becomes desaturated.

The LAYAVG value determines the method of computing interblock transmissivity.

Following are the five methods used in assigning the LAYAVG value.

- 00 Harmonic mean interblock transmissivity [Default setting for MODFLOW-96, MODFLOW-2000, and MODFLOW-2005].
- 10 Arithmetic mean interblock transmissivity.
- 20- Logarithmic mean interblock transmissivity.
- 30 Arithmetic mean saturated thickness times logarithmic mean hydraulic conductivity.
- 40 Harmonic mean interblock hydraulic conductivity introduced in BCF4 package [Default (Required) setting for MODFLOW-SURFACT].
- 50 Arithmetic mean interblock hydraulic conductivity introduced in BCF4 package.

Note that the LAYAVG values are two digits with a factor of ten. For example, a LAYCON value of 21 represents an unconfined layer where the interblock transmissivity is calculated using a logarithmic mean.

The Layer column in the Layer Settings window (see following figure) is the layer number which is automatically numbered as one row for each layer of the model grid.

The LAYCON column is the Input LAYCON value, which includes the first digit (tens) stored as the LAYAVG value (Interblock transmissivity), and the second digit (ones) stored as the LAYCON value (Layer type). Thus the one Input LAYCON value holds the identification for each layer of the model grid.

The Interblock transmissivity column displays the LAYAVG value and descriptive name associated with each layer of the model. The available LAYAVG settings can be chosen from a picklist by clicking the down arrow key, or you can scroll through the options by clicking the spin buttons on the left (as shown in the following figure).

The Layer type column displays the Layer Type associated with each layer of the model. The available layer types can be chosen from a picklist by clicking the down arrow on the right, or you can scroll through the options by clicking the spin buttons on the left.

10.10.1.8 Cell Rewetting

Settings	Translation Log	DIS	LPF	RIV	CHD	RCH	BAS	OC	PCG	NDC	LMT	IN	BT3	DP3	RC:
	aral Settings FLOW-2005 Settings Time Steps Solvers Recharge and EV Lake ayers Reveting nitial Heads Arisotropy	T	Cell w Wettir Iteratir Wettir Wettir Head Keep	ng thresh on interva ng head ng factor value in min. satu	VDFLG) d (WETD old (WET al for atter (IHDWET (WETFC	(DRY) va mpting to T) T)	lue wet cells r bottom l	: (IWETIT ayer	Fr 0.) 1 Ca 1 -1e	-			: 0) vurs (IHI	OWET =	= 0)
⊟- MT3	Dutput Control DMS Settings Solution Method Dutput Control		Cell wett Activate c												

The original USGS MODFLOW did not allow cells in unconfined layers to become resaturated if the head dropped below the bottom elevation of the grid cell during the course of the simulation or during the solution iterations. Instead, these cells were simply made inactive for the remainder of the simulation. However, the USGS later extended the Block-Centered-Flow package (BCF2) to allow for the rewetting of these "dry" cells during a transient simulation. While this represented a major advancement for more accurate representations of water table aquifers, it also causes the solution to be much more unstable in some situations. More detailed information on the cell wetting and the BCF package can be found in the MODFLOW Packages Reference Manual included with your Visual MODFLOW media, in the Manual folder.

The Re-wetting settings may be accessed by selecting MODFLOW/Re-wetting from the top menu bar of the Run section. A Dry Cell Wetting Options window will appear as shown in the following figure, and described below.

 Activate cell wetting (IWDFLG) is used to indicate if the wetting capability is active (IWDFLG = 1) or inactive (IWDFLG = 0).

- Wetting threshold is used to determine if the dry cell needs to be wetted. For a dry cell
 to become wet, the head in the adjacent grid cell(s) must be greater than the elevation
 of the bottom of the dry cell plus the Wetting threshold value.
- Wetting interval (IWETIT) indicates how often MODFLOW attempts to wet the dry cells detected during the course of the solution iterations. For example, if IWETIT = 2, cell wetting would be attempted at every second iteration. If a model with dry cells is having problems converging to a solution, it may be a result of oscillations due to drying and re-wetting of grid cells in sensitive regions of the model. Setting a larger cell wetting interval value may help the solution to converge, by allowing the heads in neighboring cells to get closer to a better solution before wetting the dry cells.

Wetting Methods

The wetting of a dry cell is triggered by the head values in adjacent grid cells (see Wetting threshold above). The Wetting method frame has two options for determining the adjacent grid cells to use for determining whether the dry cell should be wetted.

- From below (WETDRY < 0) will use only the head in the grid cell directly below the dry cell to determine if the dry cell should be wetted. This option is generally more stable, and is particularly good when the adjacent horizontal cells are poor indicators of whether a cell should become wet (e.g. areas with steep vertical gradients and variable bottom elevations).
- Wet cells from side and below (WETDRY > 0) will used the head in all four adjacent grid cells and the grid cell directly below the dry cell to determine if the dry cell should be wetted. This option is useful in situations where a dry cell is located above a no-flow cell, such that it cannot be re-wet from below. It is also applicable for one-layer models where there are no cells below. However, this method can cause some problems in multi-layer models where inactive cells occur beneath wet cells.

Wetting Head

When a dry cell is wetted, the new head may be calculated using one of two methods:

Calculated from neighbors Head = Zbot + Wetting factor * (Neighboring head – Zbot)

Calculated from threshold Head = Zbot + Wetting factor * Wetting threshold

Where Zbot is the elevation of the bottom of the current cell.

Generally, the first equation is thought to be more reasonable, since the cell's new head is varied according to the head in the neighboring cell, which caused it to become wet. However, in situations where MODFLOW is over-estimating head changes during iterations, this equation may cause non-convergence. The second equation can then be used to attempt a more stable solution.

Setting Head Values in Dry Cells

Each dry cell is assigned a default head value as a flag to indicate it is dry. This value is typically a very large negative number (e.g. -1.0e30). However, the presence of large negative head values in dry cells may cause problems for parameter estimation simulations

because this large negative value may be used to calculate the calibration residual (calculated head - observed head) at a grid cell that has become dry during one of the PEST iterations. In this case, it is more appropriate to assign the head value in dry cells equal to the cell bottom elevation to avoid this problem.

Setting Minimum Saturated Thickness

When PEST runs with varied model parameters, some of these runs may produce dry cells, and as a result MODFLOW assigns head values equal to -1.0e30 to all the dry cells. This can cause the objective function to be skewed, and the subsequent model runs to fail to converge. If the "Keep minimum saturated thickness for the bottom layer" option is activated by assigning an appropriate head value to the bottom cell, MODFLOW will keep the bottom cell saturated. It prevents the column from drying out, ensures that PEST will continue running even though the calculated head is actually below the bottom layer of the model, and helps with model convergence. It is recommended to not activate this option in the first run of a model because it is important to know if the dry cells exist or not, and by preventing the column from drying out, the model results could be misleading.

Hints For Using Dry Cell Wetting

Cell re-wetting often promotes a non-converging or unstable solution, which may be indicated by cells cycling between wet and dry. If this happens, we recommend you try the following:

- Set any cells that you know should never become wet to inactive.
- Increase the Wetting threshold value. This makes it more difficult for a cell to be wetted, and therefore helps stop MODFLOW from repeatedly turning a cell on and then off again. However, the solution may become less accurate since cells that should become wet might stay dry.
- Modify the Wetting factor value. This will increase or decrease the new head in cells which are wetted.
- Change the Wetting method that controls cell wetting.
- Change the Wetting head option that calculates the new head in the wetted cell.
- Try using the SIP or PCG solver, and modifying the solver parameters.
- For steady-state solutions, start with good initial head estimates. This will provide good indications of which cells should be wet and dry, and therefore conversions of cells between wet and dry will be minimized.

10.10.1.9 Initial Heads

In Visual MODFLOW Flex, the Initial Heads are defined at the stage of Defining the Properties. For more details, please see the section on setting <u>Initial Heads</u> in the Define Properties workflow step.

When translating your model you have the following settings for Initial Head:

Settings	Translation Log	DIS	S	LPF	RIV	CHD	RCH	BAS	OC	PCG	NDC	LMT	•
- MOD	eral Settings SFLOW-2005 Settings Time Steps Solvers Recharge and EV Lake Layers	r	4		ead optic	ons LOW Ru		se Spe	cified H	leads			
	Rewetting nitial Heads Anisotropy Dutput Control DMS Settings Solution Method Dutput Control		Use Pro Pre Run tran dire	e Specifi perties s vious M n. Warni nslation o ectory. O	step.Use ODFLOV ing: The directory. rrmake a	Is will use Ground I V Run rec selected If you sel copy of t alHeads.H	Elevation quires you .HDS file ect this o he .HDS	will use t to select cannot l ption, yo file from	t a .HDS t a .HDS be the sa u must cl the curre	tion value file from ame as th hoose a	es for the a previou e .HDS fi .HDS file	of layer us MOD le in the from and	1. Use FLOW current

- Use Specified Heads will use the values that are defined for "Initial Heads" at the Define Properties step.
- Use Ground Elevation will use the elevation values for the top of Layer 1.
- Use Previous MODFLOW Run requires you to select a .HDS file from a previous MODFLOW Run and specify the Time step to be used.

	Select previous HDS file		- 🗆 🗙
Previous HDS File			Browse
Time step			
		<u>0</u> K	<u>C</u> ancel



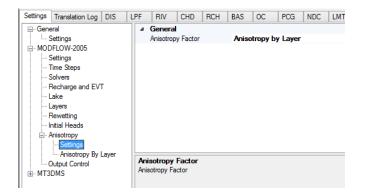
Using Heads from Previous MODFLOW Run

The selected .HDS file cannot be the same as the .HDS file in the current translation directory. If you select Use .HDS from Previous MODFLOW Run option, you must choose a .HDS file from another directory.

10.10.1.10Anisotropy

Horizontal anisotropy is the ratio of transmissivity or hydraulic conductivity along a column to its component value along each row. The Anisotropy settings in Visual MODFLOW Flex may be accessed in the Run section by selecting MODFLOW/Anisotropy from the top menu bar.

The Anisotropy Factor window (as shown in the figure below) will provide two choices for determining how the anisotropy is calculated for the model.

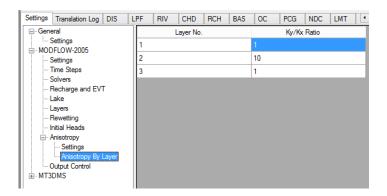


- Anisotropy by layer
- · Anisotropy as specified

The Anisotropy by layer option uses the anisotropy ratio (Ky/Kx Ratio) specified for each layer of the model (as shown in the figure), and the Kx values specified in each grid cell, to calculate the Kx or Ky values for each grid cell. Selecting Anisotropy by layer will not replace the original modeled values for Ky, but will instead calculate values during the translation of Visual MODFLOW Flex file formats to MODFLOW input data file formats to be used for the run. By default each new simulation will be set to use the Anisotropy by layer option.

The Anisotropy as specified option will use the Kx and Ky values defined for each property zone. This feature allows spatially variable anisotropy within a layer, as opposed to the Anisotropy by layer option which applies a single anisotropy ratio (Ky/Kx Factor) for the entire layer. A more in-depth discussion of spatially variable anisotropy can be found in Kladias (<u>1997</u>).

Note: MODFLOW-2000 does not support running the BCF package with Anisotropy as Specified.



10.10.1.11Output Control

The Output Control run options set the information and frequency of information written and saved to the various MODFLOW output files (see following figure).

3	Every Nth	step 1	Heads (Sav							
				S	ave to bina	ry		Print	to .LST	
	End Time	Stress Period	Time Step	Heads	DDown	F.Term	Heads	DDown	F.Term	Budget
	2.2728	1	1			\checkmark				\checkmark
	5.0003	1	2	Π	Π			Π	Π	
	8.2731	1	3							
	12.2006	1	4	Π	Π		Π	Π		
	16.9136	1	5							
	22,5691	1	6						Π	
	29.3558	1	7		Π			Π	Π	
	37.4998	1	8			v V				v V
	47.2726	1	9							⊻ ✓
	59.0	1	10							⊻ ✓
	67.2439	2	1			$\overline{\checkmark}$				
	67.2439	2	2							
	77.1365 89.0077	2	2							
	103.2531	2	4						Ц	
	120.3476	2	5							
	140.861	2	6							
	165.477	2	7							
	195.0163	2	8			\square				
	230.4634	2	9			\checkmark				\checkmark
	273.0	2	10	\checkmark	\checkmark	\checkmark				\checkmark
	276.5441	3	1			\checkmark				\checkmark
	280.797	3	2			\checkmark				\checkmark
	285.9005	3	3							\checkmark
	292.0247	3	4	Π	Π			Π	Π	
	299.3737	3	5							
	308.1926	3	6	Π	Π		Π	Π	Π	
	318.7752	3	7		Π			Π	Π	
	331.4743	3	8	Π			Π		Π	
	346.7133	3	9		Π			Π	Π	
	365.0	3	10						Π	
	367.2728	4	1		Π			Π	Π	
	370.0003	4	2							
	373.2731	4	3							
	377.2006	4	4		П					⊻ ✓
	381.9136	4	5			⊻ ✓				⊻ ✓
	387.5691	4	6			M				
	394.3558	4	° 7							
	402.4998	4	8							
	412.2726	4	9							
	424.0	4	10							
	432.2439	5	1							
	442.1365	5	2							
	454.0077	5	3							
	468 2531	5	4							

Each MODFLOW simulation can produce three binary output files and one ASCII output file:

- Binary head file (modelname.HDS)
- Binary drawdown file (modelname.DDN)
- Binary flow file (modelname.BGT)
- ASCII listing file (modelname.LST)

The binary files contain head, drawdown, and flow exchange values for each grid cell, while the ASCII listing file contains all relevant information on the operation of MODFLOW, and the simulation results. The listing (.LST) file is useful if errors occur during a simulation and you want to know how far MODFLOW progressed, or if you want to examine head or drawdown values at given intervals. For a steady-state simulation, only one set of values for each grid cell are written to these files. However, for transient simulations, each grid cell may contain simulation results for each time step, resulting in file that can become unnecessarily large. By default, the information is saved in the binary files at the end of each stress period, and at the end of the simulation in the listing (.LST) file.

The first two columns list the available stress periods and associated time steps for the entire simulation (only one stress period and time step will be listed for steady-state simulations). The remaining columns indicate the information which can be written and saved to the various MODFLOW output files. To select an output option, click in the appropriate checkbox and a checkmark (,) will appear to indicate that the selected information will be written for the selected time step.

The columns labeled Save to Binary will save the output information to the binary files as described below.

- Heads: Saves the heads in the binary heads file (.HDS).
- DDown: Saves the drawdown in the binary drawdown file (.DDN).
- F.Term: Saves the cell-by-cell flow terms in the binary budget (.BGT) file.

Please Note: The Zone Budget program uses the BGT file for calculating the flow between zones. Therefore, to change the frequency at which the Zone Budget information is saved, select the desired F.Term intervals.

The columns labeled Print to .LST will save the output information to the listing file as described below.

- Heads: Saves the heads in the listing file.
- **DDown**: Saves the drawdown in the listing file.
- F.Term: Saves the flux terms (cell by cell flow terms) in the listing file.
- Budget: Saves the budget information in the listing file.

Please Note: MODFLOW only allows the flow terms (F.Term) to be stored once, in either the binary budget file (.BGT) or the listing file (.LST). Be aware that this setting can be lost if MODFLOW is being run together with MODPATH, because MODPATH requires the flow terms to be written to the .BGT file, and not to the .LST file.

The checkbox labeled Save.FLO file will save the cell-by-cell flow terms required by MT3D/RT3D, when neither MT3D nor RT3D is being run at the same time as MODFLOW.

Saving Output Every Nth Time Step

For simulations with many stress periods and time steps, it can be very tedious to manually select the desired output time step intervals. The row of fields underneath the Output Control table are used to specify regular time step intervals for saving files during Each N-th step in each stress period. The first text box is where the N value is entered. To apply this value to the column, click the underlying checkbox.

If a subsequent engine is included in the run formation (e.g. ZoneBudget, MODPATH) with the MODFLOW simulation, Visual MODFLOW Flex will save the flow terms for all time steps by default.

10.10.1.12Advanced Settings

Advanced translation settings are available for flow simulations to enable more advanced control of translation and package settings. General and package-specific advanced settings are described below. General advanced settings are available for all Flow and Transport engines supported by Visual MODFLOW Flex, while certain engines have additional package-specific advanced settings available:

- <u>General</u>
- MODFLOW-2005/NWT
- <u>MODFLOW-SURFACT</u>

Advanced settings for SEAWAT warrant more detailed discussion and are presented separately for the <u>VDF</u> and <u>VSC</u> packages in individual sections.

Advanced Settings - General

The following settings are available for all packages:

\sim	General	
	CUnit	20
	Ext	.CHD
	LUnit	30
	Run	Yes
	Translate	Yes

- CUnit: The index for the package in the CUNIT array of the BAS file [read-only]
- Ext: The file extension of the package [read-only]
- LUnit: The file unit number to which the package will be read/written during the engine run [read-only]
- Run: Yes/No switch to determine whether the package will be added to the .NAM/.IN file and run during the simulation. **Note**: certain packages are required as part of a simulation (e.g. BAS file) and cannot be selected to not run.
- **Translate**: Yes/No switch to determine whether the package will be translated. Note: packages that do not have sufficient data will not be translated (e.g. a river package

file will not be translated if no rivers are listed in the model explorer in the active numerical model workflow).

Please Note: If a supported package is *not* represented in the model, by default it will not be translated and run, even if translate and run are both set to "Yes". For example if there are no drains represented in the model, then the DRN package will not be translated and run.

Custom/Pre-existing Input Files

If you develop or modify a package input file outside of Visual MODFLOW Flex, you can still use it as part of your modeling workflow within the Flex environment. This is particularly useful if you want to use one or more packages that are not yet supported in Visual MODFLOW Flow or if you have custom methods/utilities to generate input files. To use a custom input file:

- 1. Set Run = Yes
- 2. Set Translate = No
- Add the input file to the model run folder with the correct name and extension: [model].[ext]. The model run folder can be found by selecting the folder icon button [
], the model name will correspond to the name of your conceptual model, and the extension will be the Ext value for the package in question. For example, if you will to run the drain return package (DRT), and you are running a model where:
 - the Visual MODFLOW Flex project file is called SiteModel.amd,
 - the Conceptual Model is called Concept1,
 - the Grid is called NumericalGrid,
 - the Run is called Run 1, and
 - the Flow Engine is MODFLOW-2005

then the DRT file must be saved as:

.\SiteModel.data\MODFLOW\NumericalGrid\Run1\MODFLOW-2005\Concept1.DRT

If the above conditions are met, the custom package file will inserted into the relevant .NAM/ .IN file and run with the model. Note that certain results from unsupported packages will not be read back into Visual MODFLOW Flex, such as the flow balance terms associated with the SFR package.

Advanced Settings - MODFLOW-2005/NWT

Package-specific settings for MODFLOW-2000, -2005, and -NWT are described below:

CHD Settings

The following settings are specific to the specified head (CHD) package:

~	Misc	
	Duplicate CHD Cell Filter	Average

- **Duplicate CHD Cell Filter** When working with conceptual models, in some cases multiple constant head cells may be assigned to the same cell. When MODFLOW formulates the system of equations, it simply adds boundary conditions for all other boundary conditions this is usually not a problem as these values still require a head solution for that cell; however adding the constant head values together typically does not produce the desired result. Therefore, Visual MODFLOW Flex includes an optional filter to handle these cases on translation:
 - Minimum the minimum specified head value for the current stress period in the cell(s) with multiple values will be assigned
 - Maximum the maximum specified head value for the current stress period in the cell(s) with multiple values will be assigned
 - Average [Default] the arithmetic mean of specified head values for the current stress period in the cell(s) with multiple values will be assigned
 - Sum specified head values values for the current stress period in the cell(s) with multiple values will be added.

MNW1

The following settings are specific to the MNW1 package:

\mathbf{v}	MNW1.ltem1	
	IWELPT	No
	KSPREF	1
	NOMOITER	100
	Save Budget	Yes
~	MNW1.ltem2	
	LOSSTYPE	LINEAR
	PLossMNW	2.5
~	MNW1.ltem3.BYNODE	
	All Times	No
	BYNODE File Name	MNW1.BYNODE
	BYNODE File Unit	10002
	Write BYNODE	No
~	MNW1.ltem3.QSUM	
	All Times	No
	QSUM File Name	MNW1.QSUM
	QSUM File Unit	10003
	Write QSUM	Yes
~	MNW1.ltem3.WEL1	
	WEL1 File Name	MNW1.WEL
	WEL1 File Unit	10001
	Write WEL1	No

- **IWELPT** An integer flag used to print or omit input values from the listing file.
 - Yes Input values will be printed to the List file.
 - o No Input values will be omitted from the List file.

- **KSPER** An integer value indicating the reference stress period that will be used to calculate drawdown (typically 1).
- NOMOITER An integer representing the maximum number of iterations for determining flow in MNW cells.
- Save Buget (IWL2CB): a flag used to print or omit output flow terms to the budget (BGT) file:
 - Yes cell-by-cell flows through the MNW boundary condition will be written to the budget file
 - o No cell-by-cell flows will not be written.
- LOSSTYPE: a flag used to determine head losses between the MNW1 well and adjacent cells (see theory on <u>wells</u>, particularly Table 1):
 - $\,\circ\,$ SKIN head loss is defined with skin. Model is linear
 - o LINEAR head loss is defined with coefficient B. Model is linear
 - o NONLINEAR head loss is defined with coefficients B and C. Model is nonlinear
- BYNODE: options to write or omit an output file containing flows at each MNW well cell
- QSUM: options to write or omit an output file containing the sum of flows at each MNW cell
- WEL1: options to write or omit an output file containing the flows and heads in each MNW cell by stress period
 - (BYNODE/QSUM/WEL1) File Name: the file name to be added to the model run folder
 - All Times: a boolean flag to set which time steps will be used to output values to the (BYNODE/QSUM/WEL1) file
 - Yes values will be written at every time step
 - No values will be written based on whether flows will be written to the BGT file in the OC package
 - Write (BYNODE/QSUM/WEL1): a boolean fag to set whether the (BYNODE/QSUM/WEL1) file will be written

Note: MNW2 is mutually exclusive from MNW1.

MNW2

The following settings are specific to the MNW2 package:

\mathbf{v}	MNW2	
	MNWPRNT	Basic
	NODTOT	0
	QLimit	Transient Water Level
	Save Budget	Yes
	Vertical Wells Option	As Cells
~	MNWI.Item1.BYNODE	
	All Times	No
	BYNODE File Name	MNWI.BYNODE
	BYNODE File Unit	10002
	Write BYNODE	No
~	MNWI.Item1.QSUM	
	All Times	No
	QSUM File Name	MNWI.QSUM
	QSUM File Unit	10003
	Write QSUM	No
~	MNWI.Item 1.WEL1	
	All Times	No
	WEL1 File Name	MNWI.WEL
	WEL1 File Unit	10001
	Write WEL1	Yes
~	MNW1.ltem3	
	Data Set 3	(Collection)

- MNWPRNT Flag controlling the level of information detail about MNW wells to be written to the List file:.
 - o Basic only basic well information will be printed.
 - Standard more well information will be printed.
 - o Detailed maximum well information will be printed.
- **NODTOT** Maximum number of nodes. If NODTOT = 0, the engine will automatically estimate the maximum number of nodes.
- **QLimit** Flag that indicates whether the water level (head) in the well will be used to constrain the pumping rate:
 - o None (QLimit=0) there are no contraints on wells
 - Static Water Level (QLimit>0) pumpage will be limited by the water level in the well specified in stress period 1
 - Transient Water Level (QLimit<0) pumpage will be limited by the water level specified in each stress period
- Save Budget (IWL2CB) Flag controlling the level of information saved in the budget file:
 - Yes save budget as required by OC package
 - No do not save/print budget
 - SaveAndPrint cell-by-cell flow terms will be recorded in both the budget file and the listing file as required by the OC package. Water levels in each well will also printed to the listing file.

Notes:

- MNWI items are included in the MNW2 sections for convenience and are described in the MNWI section below.
- MNW1 is mutually exclusive from MNW2.
- MNW2 is not supported in SEAWAT

MNWI

The following settings are specific to the MNWI package:

~	MNWI.Item 1.BYNODE	
	All Times	No
	BYNODE File Name	MNWI.BYNODE
	BYNODE File Unit	10002
	Write BYNODE	No
~	MNW1.ltem1.QSUM	
	All Times	No
	QSUM File Name	MNWLQSUM
	QSUM File Unit	10003
	Write QSUM	No
\mathbf{v}	MNWI.Item1.WEL1	
	All Times	No
	WEL1 File Name	MNWI.WEL
	WEL1 File Unit	10001
	Write WEL1	Yes
~	MNW1.ltem3	
	Data Set 3	(Collection)

- BYNODE: options to write or omit an output file containing flows at each MNW well cell
- QSUM: options to write or omit an output file containing the sum of flows at each MNW cell
- WEL1: options to write or omit an output file containing the flows and heads in each MNW cell by stress period
 - (BYNODE/QSUM/WEL1) File Name: the file name to be added to the model run folder
 - All Times: a boolean flag to set which time steps will be used to output values to the (BYNODE/QSUM/WEL1) file
 - Yes values will be written at every time step
 - No values will be written based on whether flows will be written to the BGT file in the OC package
 - Write (BYNODE/QSUM/WEL1): a boolean fag to set whether the (BYNODE/QSUM/WEL1) file will be written

Notes:

• MNWI items are also included in the MNW2 sections for convenience.

OC Settings

The following settings are specific to the Output Control (OC) package:

✓ OC	
Output control file for	at type Use keywords
Use compact budget	Yes

- **Output control file format type** An integer value used to define which cell in a vertical column that recharge and discharge is simulated.
 - use codes the output control file will be generated with integer codes to that mark what output will be generated for each time step
 - use keywords [Default] the output control file will be generated with keywords that are more easily legible. This option also enables the use of the compact budget format.
- Use compact budget an optional keyword that controls the format of the output binary file
 - Yes [Default] the compact budget format will be used. This format uses less disk space than the standard format developed with MODFLOW-88
 - \circ No the standard format developed with MODFLOW-88 will be used.

Please Note: because of the expected input formats for MODPATH and MOD-PATH3DU, the OC settings will be ignored when running particle tracking simulations -MODPATH requires the code format with standard output and MOD-PATH3DU requires the use of keywords and the compact budget format.

SFR2

The following settings are specific to the SFR2 package:

SFR2.Item1a	
FACTORKH	No factor applied
Factor	1
MultiplyBy	No
FACTORKV	No factor applied
Factor	1
MultiplyBy	No
LOSSFACTOR	No factor applied
Factor	1
MultiplyBy	No
REACHINPUT	No
TRANSROUTE	No
SFR2.Item1c	
CONST	1
DLEAK	0.0001
FLWTOL	0
ISFROPT	0 - Saturated, transient
ISUZN	1
NSFRSETS	30
NSTRAIL	15
NUMTIM	10
UseKinematicWave	No
WEIGHT	0.75
	FACTORKH Factor MultiplyBy FACTORKV Factor MultiplyBy LOSSFACTOR Factor MultiplyBy REACHINPUT TRANSROUTE SFR2.Item1c CONST DLEAK FLWTOL ISFROPT ISUZN NSFRSETS NSTRAIL NUMTIM UseKinematicWave

- **FACTORKH** options to include or omit a factor for the horizontal conductivity in stream cells.
- FACTORKV options to include or omit a factor for the vertical conductivity in stream cells.
- LOSSFACTOR options to include or omit a factor to calculate seepage loss from streams.
 - o factor the factor to multiply
 - MultiplyBy a boolean fag to set whether the (FACTORKH/FACTORKV/LOSSFACTOR) file will be used
- **REACHINPUT** an optional flag that controls how SFR reaches are parameterized. When REACHINPUT is specified, variable ISFROPT (see below) is read in data set 1c. ISFROPT can be used to change the default format for entering reach and segment data or to specify that unsaturated flow beneath streams will be simulated.
 - Yes ISFROPT will be read, and unsaturated flow beneath streams may be simulated
 - No [Default] ISFROPT will not be read and unsaturated flow beneath stream segments will not be simulated.
- TRANSROUTE an optional flag that controls whether transient streamflow routing will be simulated. When TRANSROUTE is specified, optional variables IRTFLG, NUMTIM, WEIGHT, and FLWTOL will be read.
 - Yes IRTFLG, NUMTIM, WEIGHT, and FLWTOL will be read and transient streamflow routing will be simulated.
 - No [Default] transient streamflow routing will not be simulated.
- **CONST** a unit conversion constant for Manning's equation for units other than legth units in meters and time units in seconds. Note: the correct units will be included based on the project units and the values should generally be left as "1" for most circumstances.
- DLEAK A real value equal to the tolerance level of stream depth used in computing leakage between each stream reach and active model cell. Value is in units of length. Usually a value of 0.0001 is sufficient when units of feet or meters are used in model.
- **FLWTOL** A real number equal to the streamflow tolerance for convergence of the kinematic wave equation used for transient streamflow routing. A value of 0.00003 cubic meters per second has been used successfully in test simulations (and would need to be converted to whatever units are being used in the particular simulation).
- ISFROPT A flag that defines the format of the input data and whether or not unsaturated flow is simulated beneath streams. ISFROPT is only used when REACHINPUT is active.
 - Saturated, transient (0) No vertical unsaturated flow beneath streams. Streambed elevations, stream slope, streambed thickness, and streambed hydraulic conductivity are read for each stress period using variables defined in Items 6b and 6c.
 - Unsaturated, transient, constant (4) Streambed and unsaturated-zone properties are read for the beginning and end of each stream segment using variables defined in Items 6b and 6c. Streambed properties can vary each stress period. When using

the LPF Package, saturated vertical hydraulic conductivity for the unsaturated zone is the same as the vertical hydraulic conductivity of the corresponding layer in LPF and input variable UHC1 is not read.

- Unsaturated, transient, variable (5) Same as option 4 above, except saturated vertical hydraulic conductivity for the unsaturated zone (input variable UHC1) is read for each segment at the beginning of the first stress period only.
- **ISUZN** ISUZN An integer value that is the maximum number of vertical cells used to the define the unsaturated zone beneath a stream reach, the default value is 1. If ICALC is 1 for all segments then ISUZN should be set to 1.
- NSFRSETS An integer value that is the maximum number of sets of trailing waves used to allocate arrays. Arrays are allocated by multiplying NSTRAIL by NSFRSETS. A value of 30 is usually sufficient for problems where the stream depth varies often. However, in some cases a value of 50 may be required. If this value is set too small then the simulation will terminate prematurely and an error will be printed to the List file. NSFRSETS is only used when TRANSROUTE and UseKinematicWave are active
- NSTRAIL An integer value that is the number of trailing wave increments used to represent a trailing wave. Trailing waves are used to represent a decrease in the surface infiltration rate. The value can be increased to improve mass balance in the unsaturated zone. Values between 10 and 20 work well and result in unsaturated-zone mass balance errors beneath streams ranging between 0.001 and 0.01 percent. NSTRAIL is only used when TRANSROUTE and UseKinematicWave are active
- **NUMTIM** An integer value that is the number of sub time steps used to route streamflow. The time step that will be used to route streamflow will be equal to the MODFLOW time step divided by NUMTIM. NUMTIM is only used when TRANSROUTE and UseKinematicWave are active
- UseKinematicWave (IRTFLG) A flag that defines whether the kinematic wave equation will be used:
 - Yes the kinematic wave equation will be used to route streamflows and IRTFLG, NUMTIM, WEIGHT, and FLWTOL will be read
 - $\,\circ\,$ No the kinematic wave equation will not be used to route streamflows
- WEIGHT A real number equal to the time weighting factor used to calculate the change in channel storage. WEIGHT has a value between 0.5 and 1. WEIGHT is only used when TRANSROUTE and UseKinematicWave are active

Please Note: SFR2 has various levels of support depending on the flow engine used, whether MODFLOW-2000, MODFLOW-2005, or MODFLOW-NWT. Please refer to the online USGS documentation for MODFLOW. SFR2 is not supported in MODFLOW-SURFACT.

UZF Settings

The following settings are specific to the UZF package:

~	UZF1.ltem1	
	Unsaturated Zone Connection Option	1 - Layer 1
	Vertical Hydraulic Conductivity Option	2 - Kzz(sat) specified in BCF/LPF package
	Water Routing	0 - No routing
	Evapotranspiration	1 - True
	Unsaturated Budget Output Method 1	0
	Unsaturated Budget Output Method 2	0
	Number of Trailing Waves	15
	Number of Wave Sets	20
	Average Undulation Depth	1
~	UZF1.ltem8	
	Gage Cells	(Collection)

- Unsaturated Zone Connection Option (NUZOPT) An integer value used to define which cell in a vertical column that recharge and discharge is simulated.
 - 1 Recharge to and discharge from only the top model layer. This option assumes land surface is defined as top of layer 1.
 - 2 Recharge to and discharge from the specified layer in variable IUZFBND. This option assumes land surface is defined as top of layer specified in IUZFBND.
 - 3 Recharge to and discharge from the highest active cell in each vertical column. Land surface is determined as top of layer specified in IUZFBND. A constant head node intercepts any recharge and prevents deeper percolation.
- Vertical Hydraulic Conductivity Option (IUZFOPT) An integer value equal to 0, 1, or 2.
 - 0 flow will not be routed through the unsaturated zone, rather infiltration will be applied directly to the saturated zone.
 - o 1 vertical hydraulic conductivity will be specified within the UZF1 Package input file using array VKS. [not supported]
 - 2 -vertical hydraulic conductivity will be specified within either the BCF or LPF Package input file
- Water Routing (IRUNFLG) An integer value that specifies whether ground water that discharges to land surface will be routed to stream segments or lakes as specified in the IRUNBND array (IRUNFLG not equal to zero) or if ground-water discharge is removed from the model simulation and accounted for in the ground-water budget as a loss of water (IRUNFLG=0). The Streamflow-Routing (SFR2) and(or) the Lake (LAK3) Packages must be active if IRUNFLG is not zero.
- Evapotranspiration (IETFLG) An integer value that specifies whether or not evapotranspiration (ET) will be simulated. ET will not be simulated if IETFLG is zero, otherwise it will be simulated.
- Unsaturated Budget Output Method 1 (IUZFCB1) An integer value used as a flag for writing ground-water recharge, ET, and ground-water discharge to land surface rates to a separate unformatted file using subroutine UBUDSV. If IUZFCB1>0, it is the unit number to which the cell-by-cell rates will be written when "SAVE BUDGET" or a non-zero value for ICBCFL is specified in Output Control. If IUZFCB1 ≤ 0, cell-by-cell rates will not be written to a file.

- Unsaturated Budget Output Method 2 (IUZFCB2) An integer value used as a flag for writing ground-water recharge, ET, and ground-water discharge to land surface rates to a separate unformatted file using module UBDSV3. If IUZFCB2>0, it is the unit number to which cell-by-cell rates will be written when "SAVE BUDGET" or a non-zero value for ICBCFL is specified in Output Control. If IUZFCB2≤0, cell-by-cell rates will not be written to file.
- Number of Trailing Waves (NTRAIL2) An integer value equal to the number of trailing waves used to define the water-content profile following a decrease in the infiltration rate. The number of trailing waves varies depending on the problem, but a range between 10 and 20 is usually adequate. More trailing waves may decrease mass-balance error and will increase computational requirements and memory usage. This variable is not specified if IUZFOPT is zero or less.
- Number of Wave Sets (NSETS2) An integer value equal to the number of wave sets used to simulate multiple infiltration periods. The number of wave sets should be set to 20 for most problems involving time varying infiltration. The total number of waves allowed within an unsaturated zone cell is equal to NTRAIL2 * NSETS2. An error will occur if the number of waves in a cell exceeds this value. This variable is not specified if IUZFOPT is zero or less.
- Average Undulation Depth (SURFDEP) A real value equal to the average undulation depth within a finite-difference cell.

Advanced Settings - MODFLOW-SURFACT

Basic Flow (BAS) Package Settings

The following settings are specific to the BAS package:

- **IDUAL** An integer value used to define the dual-domain model for transport simulations:
 - If IDUAL=0, the simulation is for a single domain continuum.
 - If IDUAL=1, the simulation is for a dual domain representation with no equilibrium sorption occurring in the immobile domain.
 - If IDUAL=2, the simulation is for a dual domain representation with equilibrium sorption characteristics of the immobile domain being equal to that of the mobile domain at any node in the system.
 - IF IDUAL=3, the simulation is for a dual domain representation with equilibrium adsorption characteristics of the immobile domain being distinct from those of the mobile domain, requiring additional input of these properties.
- **ITRAN** An integer flag that determines if the simulation is either flow only or flow and transport.
 - \circ If ITRAN = 0, the simulation is for flow only.
 - \circ If ITRAN = 1, the simulation is for both flow and transport.

The above settings will override the Modeling Objectives selections and can be used to simplify the model without affecting the values stored in at the Modeling Objectives step or in the model explorer.

Please Note: you will likely encounter errors running the model if you select a higher value of IDUAL or ITRAN than you have set up your model to handle, for example: selecting ITRAN=1 without first having set up transport species.

Block-Centered Flow (BCF4) Package Settings

The following settings are specific to the BCF4 package:

- ATMGP Standard atmospheric pressure
- COMPAIR Compressibility of air
- COMPWATER Compressibility of water
- GRAV Gravitational acceleration constant
- IREALSL is a flag indicating which soil moisture functions are used to define flow in the unsaturated zone above the water-table:

IREALSL Pseudo-soil relations are used

= 0

Flow in the vadose is treated rigorously

> 0

groundwater flow is simulated in the vadose zone and the van

= 1 Genuchten functions are used for retention and relative permeability characteristics of the unsaturated layer(s).

groundwater flow is simulated in the vadose zone and the van

- = 2 Genuchten function is used for retention and the Brooks-Corey function is used for relative permeability characteristics of the unsaturated layer(s).
- soil vapor flow is simulated in the vadose zone and the van Genuchten
 functions are used for retention and relative permeability characteristics of the unsaturated layer(s).
- soil vapor flow is simulated in the vadose zone and the van Genuchten
 function is used for retention and the Brooks-Corey function is used for relative permeability characteristics of the unsaturated layer(s).
- RHOAP Density of air at reference pressure.
- RHOWP Density of water.
- VISG Viscosity of air.
- VISW viscosity of water

Basic Transport (BTN) Package Settings

The following settings are specific to the BTN package:

- LINR is an integer flag indicating which retardation model will be used:
 - o 0 retardation is not applied
 - o 1 linear retardation is applied
 - o 2 non-linear retardation is applied using the Freundlich isotherm sorption model

Recharge-Seepage Face (RSF4) Package Settings

The following settings are specific to the RSF4 package:

- **IUNCNF** is an integer flag for the unconfined option:
 - 0 the specified recharge (RECH) is applied always like in a confined case even if the calculated water table exceeds the top elevation in layer 1.
 - 1 Recharge seepage face boundary condition is employed and recharge (RECH) will be applied until water table reaches the ponding elevations described in PNDEL array.
- NRCHOP is an integer flag for the recharge option. Recharge rates are defined in a two-dimensional array (RECH) with one value for each vertical column. Accordingly, recharge is applied to one cell in each vertical column, and the option code determines which cell in the column is selected for recharge. NRCHOP can have the following values:
 - o 1 Recharge is only applied to the top grid layer
 - 2 Vertical distribution of recharge is specified in array IRCH [option not currently supported]
 - 3 Recharge is applied to the highest active cell in each vertical column. Note: a constant-head node intercepts recharge and prevents deeper infiltration

Time-Varying Material Properties (TMP1) Package Settings

The following settings are specific to the TMP1 package:

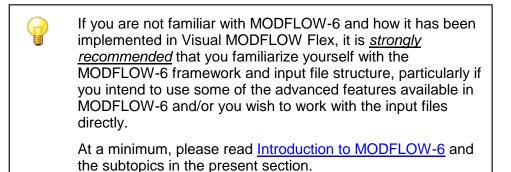
- **ICRREAD** is a switch for reading/using the vertical hydraulic conductivity (Kzz) scaling information (Cannot be used with ICVREAD).
- **ICVREAD** is a switch for reading/using the vertical leakance scaling information. (Cannot be used with ICRREAD).
- **IHYREAD** is a switch for reading/using the horizontal hydraulic conductivity (Kxx, Kyy) scaling information
- ISC1READ is a switch for reading/using the specific storage (Ss) scaling information
- ISC2READ is a switch for reading/using the specific yield (Sy) scaling information

Please Note: if ISC1READ/ISC2READ are scaled, IHYREAD is required (even if the scaling values are all set to 1).

10.10.2 MODFLOW-6

This chapter describes the features, functionality, and options in the Translation section of the Visual MODFLOW Flex interface when using MODFLOW-6 to perform the groundwater flow (GWF) simulation. The Translation section is where the MODFLOW-6 packages are generated.

Depending on the <u>Modeling Objectives</u> and if MODFLOW-6 is selected at the <u>Single Run</u> step (and associated options), the main items under the translation tree will include MODFLOW-6 and/or MODFLOW-6 <u>Transport</u>.



MODFLOW-6 Groundwater Flow Model Settings:

- General
- MODFLOW-6 Settings
- Solver Settings
- Initial Heads
- Output Control
- Advanced Settings

10.10.2.1 Introduction to MODFLOW-6

MODFLOW-6 is the latest core version of MODFLOW and represents the consolidation of a number of features that were available in separate engines, including:

- Unstructured grids (MODFLOW-USG),
- Newton-Raphson formulation (MODLFOW-NWT),
- Dual-domain solute transport (MT3D-MS),
- Multiple nested model grids (MODFLOW-LGR),

• Density-dependent flow and solute transport (SEAWAT)

as well as some new/unique features:

- full 3D anisotropy tensor support (via the XT3D formulation),
- multiple stress package instances, and
- mover/exchange packages

Note that not all of these features are supported in the latest version of Visual MODFLOW Flex; however, we will add support (based on user demand). If there is a feature of MODFLOW-6 that is not yet supported that you'd like to see added in a future version of Visual MODFLOW Flex, please let us know at support@waterloohydrogeologic.com.

MODFLOW-6 versus Previous Versions of MODFLOW

Development of previous versions of MODFLOW (e.g. MODFLOW-2000, MODFLOW-2005, MODFLOW-NWT, SEAWAT, MODFLOW-SURFACT, and MODFLOW-USG) was largely incremental in such a way that input file structure were largely consistent across versions or only required modest changes to the input structure of some input package files. Unlike these previous versions, MODFLOW-6 was completely re-written by the United States Geologic Survey staff and collaborators. As part of the re-write, the entire framework and associated structure of the input/output files are significantly different. The new input file structure is based on a pseudo-object oriented paradigm that uses keywords and a multi-model/multi-solution simulation framework. This generally makes the files more human readable; however, these changes mean that files from previous versions are not compatible with MODFLOW-6.

It is <u>strongly recommended</u> that you familiarize yourself with the MODFLOW-6 framework and input file structure, particularly if you intend to use some of the advanced features available in MODFLOW-6 and/or you wish to work with the input files directly.

Working with MODFLOW-6 in Visual MODFLOW Flex

This section highlights important differences and considerations for working MODFLOW-6 as compared to previous versions:

 MODFLOW-6 Input file formats: as described in the inset above, the input files for MODFLOW-6 are completely different from previous versions of MODFLOW. Although many of the same package names apply between previous versions of MODFLOW and MODFLOW-6, the input structures are different and in some cases packages have been replaced and/or the location of input variables has been moved into new or different packages. For example, the BAS package in older versions of MODFLOW included information about the (in)active status of grid cells (IBOUND) and starting head values (SHEAD); however, MODFLOW-6 no longer has a BAS package - grid cell status information has been included in the DIS(V) package (IDOMAIN) and the starting heads have been moved to the IC package. For more details, please refer to the input documentation for more details (USGS, <u>2022</u>).

- MODFLOW-6 Simulations: the MODFLOW-6 framework includes a new simulation level structure - this allows modelers to develop flow (and transport models) of groundwater systems in a hierarchical manner that can incorporate one or more models of the same of different types. Currently, only groundwater flow (GWF) and groundwater transport (GWT) type models are supported and the current version of Visual MODFLOW Flex has a further limitation that only one groundwater flow model and separate, but linked transport models for each species may be included in the simulation.
- Time Discretization: MODFLOW-6 includes the time discretization (TDIS) package and requires that time be discretized at the simulation level - that is information about temporal control, such as the number and duration of stress periods, the number time steps and associated multipliers are specified for the simulation as a whole rather than for each GWF/GWT model individually. This means that stress periods and time steps should be specified in a way that is suitable for all models in the simulation. If included, transport simulation typically requires finer discretization of time steps due to numerical issues associated with solving the advection-dispersion equation as reflected in the dimensionless Courant number ($C_r = v_i \Delta t / \Delta x_i$, where is v_i is the groundwater velocity in a given direction, Δt is the time step, and Δx_i is the grid spacing in that direction). Special care should be taken with selecting time steps - Courant numbers of 2 and generally no more than 5 are commonly recommended for problems involving solute transport.
- **Multi-species Transport**: MODFLOW-6 currently only supports single species transport GWT models; however, multi-species modeling in a single simulation is possible by adding a separate groundwater transport (GWT) model for each solute/species to the simulation. The GWT model does not currently support kinetic reactions between species in separate models.
- Transport Boundary Conditions: in Visual MODFLOW Flex, the default species concentrations for boundary conditions is set to -1; which previous transport engines such as MT3D-MS, RT3D, and SEAWAT interpret as zero concentrations for sources and ambient concentrations for sinks, which is particularly useful for multi-species simulation with boundary conditions where only a subset of the species have known/specified concentrations. MODFLOW-6 does not include this interpretation (likely since species concentrations are modeled independently). Currently Visual MODFLOW Flex supports transport sources/sinks in boundary conditions using AUXILIARY variables in each boundary condition along with the SSM package. To minimize discrepancies between the engines, Visual MODFLOW Flex will treat transport boundary conditions as follows during MODFLOW-6 translation:
 - If ALL concentrations of a given species in a boundary condition are negative, the boundary condition package in the GWF will omit that species as an AUXILIARY variable and omit that boundary from the SSM file in the GWT model that corresponds to that species
 - If ANY concentrations of a given species in a boundary concentrations are greater than or equal to 0, then the boundary condition package in the GWF model will

include that species as an AUXILLIARY variable and include the boundary condition in the SSM package in the GWT for that species. In this case, negative concentrations should be set to zero or the boundary condition should be split into two separate boundary conditions: one will all negative concentrations and one with all non-negative concentrations.

The exception for this is the Mass Source Loading package, which is designed to simulate solute mass fluxes that are positive (e.g. a source zone, spill, etc.) or negative (e.g. an in-situ treatment zone).

There are many more differences than those listed above, please consult the references listed below for more details and refer to the other topics in this Section about MODFLOW-6.

Recommended Reading

The following resources may be useful for learning more about MODFLOW-6:

- Official USGS MODFLOW-6 Website: <u>https://www.usgs.gov/software/modflow-6-usgs-modular-hydrologic-model</u>
- > Documentation:
 - Hughes, J.D., Langevin, C.D., and Banta, E.R., 2017, <u>Documentation for the</u> <u>MODFLOW 6 framework</u>: U.S. Geological Survey Techniques and Methods, book 6, chap. A57, 40 p., <u>https://doi.org/10.3133/tm6A57</u>.
 - Langevin, C.D., Hughes, J.D., Banta, E.R., Niswonger, R.G., Panday, Sorab, and Provost, A.M., 2017, *Documentation for the MODFLOW 6 Groundwater Flow Model*: U.S. Geological Survey Techniques and Methods, book 6, chap. A55, 197 p., <u>https://doi.org/10.3133/tm6A55</u>.
 - Langevin, C.D., Provost, A.M., Panday, Sorab, and Hughes, J.D., 2022, <u>Documentation for the MODFLOW 6 Groundwater Transport Model</u>: U.S. Geological Survey Techniques and Methods, book 6, chap. A61, 56 p., <u>https://doi.org/10.3133/tm6A61</u>.
 - United States Geological Survey, 2022. <u>MODFLOW-6 Description of Input and</u> <u>Output (Version 6.4.1)</u>. United States Geological Survey, Water and Science Availability and Use Science Program, MODFLOW 6 Development Team. Dec 2022.

10.10.2.2 General

If this node of the translation tree is selected, Visual MODFLOW Flex will display the following (read-only) information about the model simulation:

- Output folder: where the translated files will be generated.
- Start date: the start date will be the same as that which you specified in the <u>Define</u> <u>Modeling Objectives</u> step

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Settings Translation Log nam	TDIS	IMS	DIS	IC	OC	NPF	CHD	CHD(2)	RIV	WEL	nam(2)	
General Settings MODFLOW-6 Settings Solvers Initial Heads Output Control B- Advanced Settings		Genera Output I Start Da start Da	Folder te			lsers\Pub 2000	lic \Docu	ments \Visu	ial MOD	FLOW FI	lex\Tutorials\Conceptua	al Model\conceptual-model.D

10.10.2.3 MODFLOW-6 Settings

The following settings are available for the MODFLOW-6 flow engine:

Run Type: Steady-State or Transient

If the Steady-State Flow option is selected, Visual MODFLOW Flex will prepare the data set for a steady-state flow simulation, and will automatically use the data from the first time period (only) of each boundary condition and pumping well defined in Visual MODFLOW Flex to run the model to achieve flow equilibrium (i.e. a time-independent solution since all inputs are constant).

Please Note: if running a steady-state model, at least one boundary condition with a head of known elevation must be specified (e.g. constant head, river stage, drain bottom, or general head elevation).

If the Transient Flow option is selected, Visual MODFLOW Flex will prepare the data set for a transient flow simulation. During this process, Visual MODFLOW Flex will automatically merge all of the different time period data defined for each pumping well and boundary condition into the stress period format required by MODFLOW-6. This creates a time-dependent flow solution, as the model is being run with different inputs at different times.

Steady-State Simulation Time: specified time for the mass balance terms in a steady-state run.

Please Note: the settings for Property Package and Save .FLO file available for other flow engines are not applicable for MODFLOW-6. MODFLOW-6 only has one property package - the node property flow (NPF) package and the .FLO file is not necessary for MODFLOW-6 as transport as the link between flow and transport is handled through the flow model interface when running flow and transport models sequentially or through exchange package(s) if running a coupled flow and transport simulation.

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Settings Translation Log		
General	✓ General	
Settings	Run Type	Steady-State
ian MODFLOW-6	Steady-State Simulation Time	1
<mark>Settings</mark>		
···· Solvers		
Initial Heads		
Output Control		
Advanced Settings		
	Run Type	
	Simulation Type: Steady-State or Transient	
] [

Stress Periods and Time Steps

The Time Steps option is only available when you are running a transient model (i.e. when Transient Flow run type is selected). For transient flow simulations, Visual MODFLOW Flex will automatically merge all of the different time periods defined for all of the different pumping wells and boundary conditions into the uniform stress period format required by MODFLOW. A stress period is defined as a time period in which all the stresses (boundary conditions, pumping rates, etc.) on the system are constant. Unfortunately, the data collected for each modeling site is rarely synchronized in terms of stress periods, so Visual MODFLOW Flex merges the time schedules for all pumping wells and boundary conditions to determine the length of each stress period for a transient simulation. As a result, the user cannot directly modify the number of stress periods or the length of each stress period.

The Time step options window (as shown in the following figure) is used to define the number of Time steps in each stress period and the time step Multiplier is used to increment each time step size.

- General Settings MDDFLOW-6 Solvers Initial Heads Output Control ⊕ Advanced Settings	✓ General Run Type Steady-State Simu										
	Run Type Simulation Type: Stea	dy-State or Transien	t								
	Time Steps Value Stress Period	Start	End	Time Steps	Multiplier	Steady-State					
		Start 0.000	_	Time Steps	Multiplier	Steady-State					
			End			Steady-State					
	Stress Period	0.000	End 31.000	10	1.2						
	Stress Period 1 2	0.000 31.000	End 31.000 60.000	10 10	1.2 1.2						
	Stress Period 1 2	0.000 31.000 60.000	End 31.000 60.000 91.000	10 10 10	1.2 1.2 1.2						
	Stress Period 1 2 3 4	0.000 31.000 60.000 91.000	End 31.000 60.000 91.000 121.000	10 10 10 10	1.2 1.2 1.2 1.2 1.2						
	Stress Period 1 2 3 4 5	0.000 31.000 60.000 91.000 121.000	End 31.000 60.000 91.000 121.000 152.000	10 10 10 10 10 10	1.2 1.2 1.2 1.2 1.2 1.2						
	Stress Period 1 2 3 4 5 6	0.000 31.000 60.000 91.000 121.000 152.000	End 31.000 60.000 91.000 121.000 152.000 182.000	10 10 10 10 10 10 10	12 12 12 12 12 12 12 12						
	Stress Period 1 2 3 4 5 6 7	0.000 31.000 60.000 91.000 121.000 152.000 182.000	End 31.000 60.000 91.000 121.000 152.000 182.000 213.000	10 10 10 10 10 10 10 10	12 12 12 12 12 12 12 12 12						
	Stress Period 1 2 3 4 5 6 7 8	0.000 31.000 60.000 91.000 121.000 152.000 182.000 213.000	End 31.000 60.000 91.000 121.000 152.000 182.000 213.000 244.000	10 10 10 10 10 10 10 10 10	1.2 1.2 1.2 1.2 1.2 1.2 1.2 1.2 1.2 1.2						
	Stress Period	0.000 31.000 60.000 91.000 121.000 152.000 182.000 213.000 244.000	End 31.000 60.000 91.000 121.000 152.000 182.000 213.000 244.000 274.000	10 10 10 10 10 10 10 10 10 10	1.2 1.2 1.2 1.2 1.2 1.2 1.2 1.2 1.2 1.2						

The Stress Period column indicates the stress period number while the Start and End columns indicate the start time and end time, respectively, for each stress period.

Each stress period is divided into a user-defined number of Time steps whereby the model will calculate the head solution at each time step. The default value for Time steps is 10.

The time step Multiplier is the factor used to increment the time step size within each stress period (i.e. it is the ratio of the value of each time step to that of the preceding time step). The default value is 1.2. A time step Multiplier value greater than 1 will produce smaller time steps at the beginning of a stress period resulting in a better representation of the changes of the transient flow field. Thus increasing the number of time steps in a simulation may result in smoother head or drawdown versus time curves.

The steady-state column indicates if the stress period is transient or steady-state. This setting allows individual stress periods in a single simulation to be either transient or steady state instead of requiring the entire simulation to be either steady state or transient. Steady-state and transient stress periods can occur in any order. Commonly the first stress period may be run as steady state, to produce a solution that is used as the initial condition for subsequent transient stress periods.

Accommodating Boundary Conditions with Varying End Times

Visual MODFLOW Flex allows you to define boundary conditions with varying end times; the number of stress periods for the model will be calculated from the end time of the longest boundary condition. If there is a stress period where there are no data defined for a boundary condition, then you will see an entry of "0" in the appropriate package, for that

stress period; this denotes that zero cells are defined for that stress period. In the case of pumping wells, you will see a rate of 0 for the well cells.

10.10.2.4 Solver Settings

Solvers in MODFLOW-6 are handled through the iterative model solution (IMS) package which is used to solve flow and/or transport simulations. The IMS package uses a linear and non-linear methods to solve the simultaneous equations produced by the model(s) as described below:

ttings Translation Log nam	TDIS	IMS DIS IC OC NPF	CHD CHD(2) RIV WEL STO nam(2)						
⊡ General		General							
Settings		Selected Solver	Iterative Matrix Solver (IMS)						
MODFLOW-6									
Settings									
Solvers									
Initial Heads		Options							
Output Control		PrintOption	None						
Advanced Settings MODFLOW-6 Transport-Specific General		Complexity	Simple						
		CsvOuterOutput	False						
		CsvInnerOutput	False						
Solvers		NoPtc	First						
Initial Concentrations		AtsOuterMaximumFraction	0.25						
Output Control	~	Linear							
Advanced Settings		InnerMaximum	100						
		InnerDVClose	1E-06						
		InnerRClose	1E-06						
		LinearAcceleration	BICGStab						
		RelaxationFactor	0						
		PreconditionerLevels	0						
		PreconditionerDrop Tolerance	0						
		NumberOrthogonalizations	0						
		ScalingMethod	None						
		ReorderingMethod	None						
	~	Nonlinear							
		OuterDVClose	0.01						
		OuterMaximum	100						
		UnderRelaxation	None						
		UnderRelaxationGamma	0.2						
		UnderRelaxation Theta	0.7						
		UnderRelaxationKappa	0.1						
		UnderRelaxationMomentum	0.001						
		BacktrackingNumber	10						
		BacktrackingTolerance	10000						
		BacktrackingReductionFactor	0.2						
		BacktrackingResidualLimit	100						
	A me re	sidual reduction summaries. ALL means print	iomation from the solver. NONE only the total number of iterations and nonlinear linear matrix solver convergence information to the trix solver convergence information to each model						

General Solution Options

The following settings are optional in the IMS package:

- PrintOption: An optional keyword setting that determines the print level of the solver in the listing file:
 - Summary means print only the total number of iterations and nonlinear residual reduction summaries.
 - All means print linear matrix solver convergence information to the solution listing file and model specific linear matrix solver convergence information to each model listing file in addition to *Summary* information.
 - *None* means that no solver information will be printed. This is the default option.
- Complexity: is an optional keyword that defines default non-linear and linear solver parameters.
 - Simple indicates that default solver input values will be defined that work well for nearly linear models. This option is generally suitable for models that do not include nonlinear stress packages and models that are either confined or consist of a single unconfined layer that is thick enough to contain the water table within a single layer.
 - Moderate: indicates that default solver input values will be defined that work well for moderately nonlinear models. This option is generally suited for models that include nonlinear stress packages and models that consist of one or more unconfined layers. The *Moderate* option should be used when the *Simple* option does not result in successful convergence.
 - Complex: indicates that default solver input values will be defined that work well for highly nonlinear models. This option is generally suited for models that include nonlinear stress packages and models that consist of one or more unconfined layers representing complex geology and surface-water/groundwater interaction. The complex option should be used when the moderate option does not result in successful convergence.
 - Custom: indicates that custom values will be defined for the linear and non-linear solvers.

If the Simple, Moderate, or Complex options are selected, then only the items in the linear and non-linear solver sections below marked with * will be translated. All other options will use the defaults below:

SETTINGS	COMPLEXITY							
SETTINGS	SIMPLE	COMPLEX						
NON-LINEAR SOLVER SE	TTINGS							
OUTER_DVCLOSE *	0.001	0.01	0.1					
OUTER_MAXIMUM *	25	50	100					
UNDER_RELAXATION	NONE	DBD	DBD					
UNDER_RELAXATION_TH ETA	1	0.9	0.8					

UNDER_RELAXATION_KA PPA	0	0.0001	0.0001
UNDER_RELAXATION_G AMMA	0	0	0
UNDER_RELAXATION_M OMENTUM	0	0	0
BACKTRACKING_NUMBE R	0	0	20
BACKTRACKING_TOLER ANCE	0	0	1.05
BACKTRACKING_REDUC TION_FACTOR	0	0	0.1
BACKTRACKING_RESIDU AL_LIMIT	0	0	0.002
LINEAR SOLVER SETTING	S		
INNER_MAXIMUM *	50	100	500
INNER_DVCLOSE *	0.001	0.01	0.1
INNER_RCLOSE *	0.1	0.1	0.1
RCLOSE_OPTION	infinity-norm	infinity-norm	infinity-norm
LINEAR_ACCELERATION	CG	BICGSTAB	BICGSTAB
RELAXATION_FACTOR	0	0.97	0
PRECONDITIONER_LEVE LS	0	0	5
PRECONDITIONER_DRO P_TOLERANCE	0	0	0.0001
NUMBER_ORTHOGONALI ZATIONS	0	0	2
SCALING_METHOD	NONE	NONE	NONE
REORDERING_METHOD	NONE	NONE	NONE

- **CsvOuterOutput**: if this option is set to yes, then outer iteration convergence information will be written to a comma separated values file in the GWF subfolder. This option is off by default. Information written to this file includes maximum dependent-variable (for example, head or concentration) change convergence information at the end of each outer iteration for each time step.
- CsvInnerOutput: if this option is set to yes, then inner iteration convergence information will be written to a comma separated values file in the GWF subfolder. This

option is off by default. Information written to this file includes maximum dependentvariable (for example, head or concentration) change and maximum residual convergence information for the solution and each model (if the solution includes more than one model) and linear acceleration information for each inner iteration.

- NoPTC: is a settings that is used to control the pseudo-transient continuation (PTC) options for steady state periods for models using the Newton-Raphson formulation (which is controlled by in NAM file <u>settings</u>):
 - o None: PTC will not be used in solution
 - o First: PTC will be activated for the first stress period
 - o All: PTC will be deactivated for all stress periods

For many problems, PTC can significantly improve convergence behavior for steadystate simulations, and for this reason it is active by default. In some cases; however, PTC can worsen the convergence behavior, especially when the initial conditions are similar to the solution. When the initial conditions are similar to (or exactly the same as) the solution and convergence is slow, then the NO_PTC FIRST option should be used to deactivate PTC for the first stress period. The NO_PTC ALL option should also be used in order to compare convergence behavior with other MODFLOW versions, as PTC is only available in MODFLOW 6.

• AtsOuterMaximumFraction: real value defining the fraction of the maximum allowable outer iterations used with the Adaptive Time Step (ATS) capability if it is active. If this value is set to zero by the user, then this solution will have no effect on ATS behavior. This value must be greater than or equal to zero and less than or equal to 0.5 or the program will terminate with an error. If it is not specified by the user, then it is assigned a default value of one third. When the number of outer iterations for this solution is less than the product of this value and the maximum allowable outer iterations, then ATS will increase the time step length by a factor of DTADJ in the ATS input file. When the number of outer iterations for this solution is greater than the maximum allowable outer iterations, then ATS (if active) will decrease the time step length by a factor of 1 / DTADJ.

Non-Linear Solver Options

The following settings are available for the Non-linear solver:

- **OUTER_DVCLOSE**: real value defining the dependent-variable (for example, head or concentration) change criterion for convergence of the outer (nonlinear) iterations, in units of the dependent-variable (for example, length for head or mass per length cubed for concentrations). When the maximum absolute value of the dependent-variable change at all nodes during an iteration is less than or equal to OUTER_DVCLOSE, iteration stops.
- **OUTER_MAXIMUM**: integer value defining the maximum number of outer (nonlinear) iterations. For a linear problem OUTER_MAXIMUM should be 1.

- UNDER_RELAXATION: an optional keyword that defines the nonlinear underrelaxation schemes used. Under-relaxation is also known as dampening, and is used to reduce the size of the calculated dependent variable before proceeding to the next outer iteration. Under-relaxation can be an effective tool for highly nonlinear models when there are large and often counteracting changes in the calculated dependent variable between successive outer iterations. By default under-relaxation is not used.
 - o NONE [Default] under-relaxation is not used
 - *SIMPLE* Simple under-relaxation scheme with a fixed relaxation factor (*under relaxation gamma* (see below)) is used.
 - o COOLEY Cooley under-relaxation scheme is used.
 - o DBD delta-bar-delta (DBD) under-relaxation is used.

Note that the under-relaxation schemes are often used in conjunction with problems that use the Newton-Raphson formulation (which is controlled by in NAM file <u>settings</u>); however, experience has indicated that they also work well for non-Newton problems, such as those with the wet/dry options of MODFLOW 6.

- UNDER RELAXATION GAMMA: a real value defining either the relaxation factor for the simple complexity scheme or the history or memory term factor of the Cooley and delta-bar-delta algorithms. For the simple scheme, a value of one indicates that there is no under-relaxation and the full head (or concentration) change is applied. This value can be gradually reduced from one as a way to improve convergence; for well behaved problems, using a value less than one can increase the number of outer iterations required for convergence and needlessly increase run times. Under relaxation gamma must be greater than zero for the simple scheme or the program will terminate with an error. For the Cooley and delta-bar-delta schemes, Under relaxation gamma is a memory term that can range between zero and one. When Under relaxation gamma is zero, only the most recent history (previous iteration value) is maintained. As Under relaxation gamma is increased, past history of iteration changes has greater influence on the memory term. The memory term is maintained as an exponential average of past changes. Retaining some past history can overcome granular behavior in the calculated function surface and therefore helps to overcome cyclic patterns of non-convergence. The value usually ranges from 0.1 to 0.3; a value of 0.2 works well for most problems. Under relaxation gamma is only used in the simulation if Under relaxation is not None.
- UNDER_RELAXATION_THETA: a real value defining the reduction factor for the learning rate (underrelaxation term) of the delta-bar-delta algorithm. The value of *under relaxation theta* is between zero and one. If the change in the dependent-variable (for example, head or concentration) is of opposite sign to that of the previous iteration, the under-relaxation term is reduced by a factor of *under relaxation theta*. The value usually ranges from 0.3 to 0.9; a value of 0.7 works well for most problems. *Under relaxation theta* is only used in the simulation if *under relaxation* is DBD.
- UNDER_RELAXATION_KAPPA: a real value defining the increment for the learning rate (under-relaxation term) of the delta-bar-delta algorithm. The value of *under relaxation kappa* is between zero and one. If the change in the dependent-variable (for example, head or concentration) is of the same sign to that of the previous iteration, the under-relaxation term is increased by an increment of *under relaxation kappa*. The

value usually ranges from 0.03 to 0.3; a value of 0.1 works well for most problems. *Under relaxation kappa* is only used in the simulation if *under relaxation* is DBD.

- UNDER_RELAXATION_MOMENTUM: a real value defining the fraction of past history changes that is added as a momentum term to the step change for a nonlinear iteration. The value of *under relaxation momentum* is between zero and one. A large momentum term should only be used when small learning rates are expected. Small amounts of the momentum term help convergence. The value usually ranges from 0.0001 to 0.1; a value of 0.001 works well for most problems. *Under relaxation momentum* is only used in the simulation if *under relaxation* is DBD.
- **BACKTRACKING_NUMBER**: an integer value defining the maximum number of backtracking iterations allowed for residual reduction computations. If *backtracking number* = 0 then the backtracking iterations are omitted. The value usually ranges from 2 to 20; a value of 10 works well for most problems.
- **BACKTRACKING_TOLERANCE**: a real value defining the tolerance for residual change that is allowed for residual reduction computations. The *backtracking tolerance* value should not be less than one to avoid getting stuck in local minima. A large value serves to check for extreme residual increases, while a low value serves to control step size more severely. The value usually ranges from 1.0 to 106; a value of 104 works well for most problems but lower values like 1.1 may be required for harder problems. *Backtracking tolerance* is only used in the simulation if *backtracking number* is greater than zero.
- **BACKTRACKING_REDUCTION_FACTOR**: real value defining the reduction in step size used for residual reduction computations. The value of is between zero and one. The value usually ranges from 0.1 to 0.3; a value of 0.2 works well for most problems. *Backtracking reduction factor* is only used in the simulation if *backtracking number* is greater than zero.
- **BACKTRACKING_RESIDUAL_LIMIT**: a real value defining the limit to which the residual is reduced with backtracking. If the residual is smaller than *backtracking residual limit*, then further backtracking is not performed. A value of 100 is suitable for large problems and residual reduction to smaller values may only slow down computations. *Backtracking residual limit* is used in the simulation if *backtracking number* is greater than zero.

Linear Solver Options

The following settings are available for the Linear solver:

- **INNER_MAXIMUM**: an integer value defining the maximum number of inner (linear) iterations. The number typically depends on the characteristics of the matrix solution scheme being used. For nonlinear problems, *inner maximum* usually ranges from 60 to 600; a value of 100 will be sufficient for most linear problems.
- **INNER_DVCLOSE**: a real value defining the dependent-variable (for example, head or concentration) change criterion for convergence of the inner (linear) iterations, in units of the dependent-variable (for example, length for head or mass per length cubed for

∆h ≤ concentration). When the maximum absolute value of the dependent-variable change at all nodes during an iteration is less than or equal to *inner dvclose*, the matrix solver assumes convergence. Commonly, *inner_dvclose* is set equal to or an order of magnitude less than the *outer_dvclose* value specified for the non-linear block.

- **INNER_RCLOSE**: a real value that defines the flow residual tolerance for convergence of the IMS linear solver and specific flow residual criteria used. This value represents the maximum allowable residual at any single node. Value is in units of length cubed per time, and must be consistent with MODFLOW-6 length and time units. Usually a value of 0.1 is sufficient for the flow-residual criteria when meters and seconds are the defined MODFLOW-6 length and time.
- RCLOSE_OPTION: an optional keyword that defines the specific flow residual criterion used.
 - STRICT: an optional keyword that is used to specify that *inner rclose* represents a infinity-Norm (absolute convergence criteria) and that the dependent-variable (for example, head or concentration) and flow convergence criteria must be met on the first inner iteration (this criteria is equivalent to the criteria used by the MODFLOW-2005 PCG package (Hill, <u>1990</u>)).
 - L2NORM_RCLOSE: an optional keyword that is used to specify that *inner rclose* represents a L-2 Norm closure criteria instead of a infinity-Norm (absolute convergence criteria). When *L2norm rclose* is specified, a reasonable initial *inner rclose* value is 0.1 times the number of active cells when meters and seconds are the defined MODFLOW-6 length and time.
 - RELATIVE_RCLOSE: an optional keyword that is used to specify that *inner rclose* represents a relative L-2 Norm reduction closure criteria instead of a infinity-Norm (absolute convergence criteria). When *relative rclose* is specified, a reasonable initial *inner rclose* value is 1.0×10⁻⁴ and convergence is achieved for a given inner (linear) iteration when *inner dvclose* and the current L-2 Norm is ≤ the product of the *relative_rclose* and the initial L-2 Norm for the current inner (linear) iteration. If *rclose option* is not specified, an absolute residual (infinity-norm) criterion is used.
- LINEAR ACCELERATION: a keyword that defines the linear acceleration method used by the default IMS linear solvers.
 - o CG preconditioned conjugate gradient method.
 - o BICGSTAB preconditioned bi-conjugate gradient stabilized method.
- **RELAXATION_FACTOR**: an optional real value that defines the relaxation factor used by the incomplete LU factorization preconditioners (MILU(0) and MILUT). *Relaxation_factor* is unitless and should be greater than or equal to 0.0 and less than or equal to 1.0. *Relaxation factor* values of about 1.0 are commonly used, and experience suggests that convergence can be optimized in some cases with relax values of 0.97. A *Relaxation factor* value of 0.0 will result in either ILU(0) or ILUT preconditioning (depending on the value specified for *preconditioner levels* and/or *preconditioner drop tolerance*). By default, *relaxation factor* is zero.
- **PRECONDITIONER_LEVELS**: an optional integer value defining the level of fill for ILU decomposition used in the ILUT and MILUT preconditioners. Higher levels of fill provide more robustness but also require more memory. For optimal performance, it is

suggested that a large level of fill be applied (7 or 8) with use of a drop tolerance. Specification of a *preconditioner levels* value greater than zero results in use of the ILUT preconditioner. By default, the number of *preconditioner levels* is zero and the zero-fill incomplete LU factorization preconditioners (ILU(0) and MILU(0)) are used.

- **PRECONDITIONER_DROP_TOLERANCE**: a real value that defines the drop tolerance used to drop preconditioner terms based on the magnitude of matrix entries in the ILUT and MILUT preconditioners. A value of 10⁻⁴ works well for most problems. By default, the *preconditioner drop tolerance* is zero and the zero-fill incomplete LU factorization preconditioners (ILU(0) and MILU(0)) are used.
- NUMBER_ORTHOGONALIZATIONS: an integer value defining the interval used to explicitly recalculate the residual of the flow equation using the solver coefficient matrix, the latest dependent/variable (for example, head or concentration) estimates, and the right hand side. For problems that benefit from explicit recalculation of the residual, a number between 4 and 10 is appropriate. By default, the *number of orthogonalizations* is zero.
- SCALING_METHOD: an optional keyword that defines the matrix scaling approach used. By default, matrix scaling is not applied.
 - NONE [Default] no matrix scaling applied.
 - DIAGONAL symmetric matrix scaling using the POLCG preconditioner scaling method in Hill (<u>1990</u>).
 - o L2NORM symmetric matrix scaling using the L-2 Norm.
- **REODERING_METHOD**: an optional keyword that defines the matrix reordering approach used. By default, matrix reordering is not applied.
 - o NONE [Default] original ordering.
 - o RCM reverse Cuthill McKee ordering.
 - o *MD* minimum degree ordering.

10.10.2.5 Initial Heads

In Visual MODFLOW Flex, the Initial Heads are defined at the stage of Defining the Properties. For more details, please see the section on setting <u>Initial Heads</u> in the Define Properties workflow step.

When translating your model you have the following settings for Initial Head:

🔄 🗇 🙆 🔊		
Settings Translation Log		
- General - Settings - MODFLOW-6 - Settings - Solvers - Initial Heads - Output Control - Difference in the setting of the s	General Initial head options Previous MODFLOW Run HDS file	Use Ground Elevation C:\Users\Public\Documents\Visual MODFLOW Flex\Tutoria
⊕- Advanced Settings	Elevation will use the elevation values for the of a previous MODFLOW Run. Warning: The sel- directory. If you select this option, you must cho	e defined for "Initial Heads" at the Define Properties step. Use Ground f layer 1. Use Previous MODFLOW Run requires you to select a .HDS file from ected .HDS file cannot be the same as the .HDS file in the current translation ose a .HDS file from another directory. Or make a copy of the .HDS file from . Model_InitialHeads.HDS), and choose this file.

- Use Specified Heads will use the values that are defined for "Initial Heads" at the Define Properties step.
- Use Ground Elevation will use the elevation values for the top of Layer 1.
- Use Previous MODFLOW Run requires you to select a .HDS file from a previous MODFLOW Run and specify the Time step to be used. The .HDS file must be based on the same grid type and number of cells in each applicable dimension (i.e. layer, row, and columns for a structured grid, and same number of layers and cells per layer for an unstructured grid)

	Select previous HDS file	- 🗆 🗙
Previous HDS File		Browse
Time step ✓		

Warning! Warning! Using Heads from Previous MODFLOW Run The selected .HDS file cannot be the same as the .HDS file in the current translation directory. If you select Use .HDS from Previous MODFLOW Run option, you must choose a .HDS file from another directory.

10.10.2.6 Output Control

The Output Control options set the information and frequency of information written and saved to the MODFLOW-6 output files (see following figure).

Define Properties Define Boundary Conditions	Settings Translation Log nam	TDIS IMS (DIS IC OO	NPF C	HD RIV	/ RIV(2)	WEL W	/EL(2) RC	H EVT	nam(2)	
Select the Next Step Define Observations	- General	🗭 Every Nth	n step 1	Heads (Sav	e to binaŋ	n -					
Define Observations	Settings					Save to bin	arv		Print	to LST	
Define Particles	Settings	End Time	Stress Period	Time Step	Heads	DDown	F Term	Heads	DDown	F.Term	Budget
- Select Run Type	Solvers		Stress Feriod	Time Step		DDown					-
PEST Run	Initial Heads	1.1942	1	1							
Single Run	Output Control	2.6273	1	2	<u> </u>			<u> </u>			
Translate	Advanced Settings	4.3469	1	3	Ц			Ц			
Run Numerical Engines		6.4105	1	4	님			<u> </u>			
View Results		8.8868	1	5	Ц	Ц		Ц			
- View Charts		11.8584	1	6	님						
📓 View Maps		15.4242	1	7	Ц			Ц			
		19.7033		8	<u>Ц</u>			<u> </u>			
		24.8382		9							
		31.0		10							
		32.1172	2	1							
		33.4578	2	2			\checkmark				
		35.0665	2	3							
		36.9969	2	4			\checkmark				
		39.3135	2	5							
		42.0933	2	6							
		45.4291	2	7							
		49.4321		8							
		54.2357		9							
		60.0		10							
		61,1942	3	1							\checkmark

By default, each MODFLOW-6 groundwater flow model simulation will produce several output files as described below. The Output Control settings allow you to specify the stress period(s)/time step(s) for which model results of interest will be written to these output files. The Output Control Settings are provided in a tabular format based on the transient settings in the MODFLOW-6 Settings tab:

• Schedule:

- End Time: the elapsed simulation time corresponding to the end of the specified stress period and time step
- o Stress Period: the stress period in the schedule
- Time Step: the time step within the stress period
- Save to Binary:
 - Heads: simulated heads will be written to the binary heads file (.
 \GWE\modelname HDS) for active cells in the grid for selected End Time
 - \GWF\modelname.HDS) for active cells in the grid for selected End Times (Stress Period/Time Step)
 - DDown: drawdown values (i.e. the simulated head minus the initial head) will be written to the binary heads file (.\GWF\modelname.DDN) for active cells in the grid for selected End Times (Stress Period/Time Step).

Please Note: when selecting drawdown output for a given End Time (Stress Period/Time Step), the head outputs must also be selected. This is due to the fact that unlike previous versions of MODFLOW, MODFLOW-6 does not produce this file natively and drawdowns are generated by Visual MODFLOW Flex as post-processing step from the output heads.

• **F. Term**: flow budget terms, sometimes called cell-by-cell and boundary condition flow terms, will be written to the binary budget file (.\GWF\modelname.BGT) for active cells and boundary conditions in the grid for selected End Times (Stress Period/Time Step). The budget information is used to generate the budget and velocity outputs in Visual MODFLOW Flex.

Please Note: for cell-by-cell values to be added to the budget file, the SAVE_FLOWS option must be enabled (set to "Yes") in the Advanced Settings for the NAM package. Similarly, for cell-to-boundary condition values to be added to the budget file, the SAVE_FLOWS option must be enabled in the Advanced Settings for each desired boundary condition. In Visual MODFLOW Flex, the SAVE_FLOWS option is enabled by default for all supported packages including the NAM file and supported boundary conditions.

- **Print to LST:** information will be written to the listing file (.\GWF\modelname.LST):
 - Heads: simulated heads will be written to the listing file for active cells in the grid for selected End Times (Stress Period/Time Step). Note that this option should be used sparingly, typically for model troubleshooting, particularly as this format can lead to overly large output files that are less efficient to work with than the binary file or related files that can be exported from Visual MODFLOW Flex.
 - F. Term: flow budget terms, sometimes called cell-by-cell and boundary condition flow terms, will be written to listing file for active cells and boundary conditions in the grid for selected End Times (Stress Period/Time Step). Note that this option should be used sparingly, typically for model troubleshooting, particularly as this format can lead to overly large output files that are less efficient to work with than the binary file or related files that can be exported from Visual MODFLOW Flex.
 - Budget: net flow budget terms, expressed at a package level, for boundary conditions and internal storage will be written to the listing file for selected End Times (Stress Period/Time Step)

Please Note: for cell-by-cell values to be added to the listing file, the PRINT_FLOWS option must be enabled (set to "Yes") in the Advanced Settings for the NAM package. Similarly, for cell-to-boundary condition values to be added to the budget file, the PRINT_FLOWS option must be enabled in the Advanced Settings for each desired boundary condition. In Visual MODFLOW Flex, the PRINT_FLOWS option is enabled by default for all supported packages including the NAM file and supported boundary conditions.

Saving Output Every Nth Time Step

For simulations with many stress periods and time steps, it can be very tedious to manually select the desired output time step intervals. The row of fields underneath the Output Control table are used to specify regular time step intervals for saving files during Each N-th step in each stress period. The first text box is where the N value is entered. To apply this value to the column, click the underlying checkbox.

If a subsequent engine is included in the run formation (e.g. ZoneBudget) with the MODFLOW simulation, Visual MODFLOW Flex will save the flow terms for all time steps by default.

10.10.2.7 Advanced Settings

Advanced translation settings are available for flow simulations to enable more advanced control of translation and package settings. General and package-specific advanced settings are described below. General advanced settings are available for all Flow and Transport engines supported by Visual MODFLOW Flex, while certain engines have additional package-specific advanced settings available:

- General
- <u>Common Options</u>
- MODFLOW-6 Flow Packages

General

The following settings are available for all packages:

✓ General		
Ext	.TDIS	
Run	Yes	
Translate	Yes	

- Ext: The file extension of the package [read-only]
- Run: Yes/No switch to determine whether the package will be added to the .NAM file and run during the simulation. Note: certain packages are required as part of a simulation (e.g. MFSIM, TDIS, IMS, NAM, IC, OC, and NPF files) and cannot be selected to not run.
- **Translate**: Yes/No switch to determine whether the package will be translated. **Note:** If a supported package is *not* represented in the model, it will not be translated and run by default, even if translate and run are both set to "Yes". For example, if there are no drains represented in the model, then the DRN package will not be translated and run.

How to Use Custom/Pre-existing Input Files
If you develop or modify a package input file outside of Visual MODFLOW Flex, you can still use it as part of your modeling workflow within the Flex environment. This is particularly useful if you want to use one or more packages that are not yet supported in Visual MODFLOW Flow or if you have custom methods/utilities to generate input files. To use a custom input file:
1. Set Run = Yes
2. Set Translate = No

- 3. Add the input file to the model run folder with the correct name and extension: [model].[ext]. The model run folder can be found by selecting the folder icon button [⁽¹⁾], the flow model for a MODFLOW-6 model will be stored in the .\GWF subfolder, the model name will correspond to the name of your conceptual model, and the extension will be the **Ext** value for the package in question. For example, if you will to run the horizontal flow barrier package (HFB), and you are running a model where:
 - the Visual MODFLOW Flex project file is called SiteModel.amd,
 - the Conceptual Model is called Concept1,
 - the Grid is called NumericalGrid,
 - the Run is called Run 1, and
 - the Flow Engine is MODFLOW-6

then the HFB file must be saved as: .\SiteModel.data\MODFLOW\NumericalGrid\Run1\MODFLOW-6\GWF\Concept1.DRT

If the above conditions are met, the custom package file will inserted into the relevant .NAM file and run with the model. Note that certain results from unsupported packages will not be read back into Visual MODFLOW Flex, such as the flow balance terms associated with the SFR package.

Common Options

The following settings are available for the options block in many packages:

~ C	PTIONS	
В	OUNDNAMES	Yes
N	lover	No
P	RINT_FLOWS	No
P	RINT_INPUT	No
S	AVE_FLOWS	Yes
U	Jse as Obs Targets	No
U	Jse Time Series	No

• **Boundnames**: Yes/No switch to indicate whether or not boundnames will be used. If set to yes, then the name(s) of the boundary condition(s) of the given type will be added as boundnames to the package file and MODFLOW-6 will track flows and

volumes in the mass budget separately for these boundaries. The Boundnames option is set to yes by default.

- PRINT_FLOWS: Yes/No switch to indicate whether the list of flow rates through the given package type will be printed to the listing file for every stress period time step for which the Print to .LST > Budget is selected in the <u>Output Control</u> settings.The PRINT_FLOWS option is set to yes by default.
- SAVE_FLOWS: Yes/No switch to indicate whether cell-by-cell flow rates through the given package type will be written to the budget file for every stress period time step for which the Save to Binary > Budget is selected in the <u>Output Control</u> settings.The SAVE_FLOWS option is set to yes by default.

Additional options (e.g. Mover, Use as Obs Targets, Use Time Series) are included as readonly options. Support for these options will be added in future versions of Visual MODFLOW Flex. In the meantime, these options may be included in the simulation through manual edits to translated files. For more details please refer to the MODFLOW-6 Description of Input and Output manual (USGS, <u>2022</u>).

MODFLOW-6 - Flow Packages

Package-specific settings for MODFLOW-6 flow model packages are described below:

NPF Settings

The following settings are specific to the node property flow (NFP) package:

×	General	
	Ext	.NPF
	Run	Yes
	Translate	Yes
~	GRIDDATA	
	ANGLE1	(Collection)
	ANGLE2	(Collection)
	ANGLE3	(Collection)
¥	OPTIONS	
	ALTERNATIVE_CELL_AVERAGING	AMT_HMK
	AnglesByCell	No
	CellType	ByLayer
	DEWATERED	No
	PERCHED	No
	SAVE_FLOWS	Yes
	SAVE_SATURATION	No
	SAVE_SPECIFIC_DISCHARGE	No
	THICKSTRT	No
	TVK6	No
	VARIABLECV	No
	WETDRY	Global
	XT3D	None

Options

- Alternative Cell Averaging This setting allows you to select how MODFLOW-6 will calculate intercell conductance:
 - AMT_HMK [Default]: is "arithmetic-mean thickness and harmonic-mean hydraulic conductivity" method of computing transmissivity
 - AMT_LMK: is "arithmetic-mean thickness and logarithmic-mean hydraulic conductivity" method of computing transmissivity (assumes the aquifer is flat with a water table in which hydraulic conductivity varies linearly between nodes);
 - Logarithmic: is "logarithmic-mean" method (assumes transmissivity varies linearly between nodes);
- **DEWATERED** If the *dewatered* option is set to yes, then the vertical conductance is calculated using only the saturated thickness and properties of the overlying cell if the head in the underlying cell is below its top. The *dewatered* option is off by default.
- **PERCHED** If the *perched* option is set to yes, when a cell is overlying a dewatered convertible cell (see option above), the head difference used in Darcy's Law is equal to the head in the overlying cell minus the bottom elevation of the overlying cell. If not specified, then the default is to use the head difference between the two cells. The *perched* option is off by default.
- SAVE_SATURATION If the SAVE_SATURATION option is set to yes, the cell saturation will be written as a term in the budget file, for every stress period time step for which the Save to Binary > Budget is selected in the <u>Output Control</u> settings. The SAVE_SATURATION option is set to no by default.

- SAVE_SPECIFIC_DISCHARGE If the SAVE_SPECIFIC_DISCHARGE option is set to yes, then MODFLOW-6 will calculate the x, y, and z components of specific discharge (at cell centers) and write the values to the budget file, for every stress period time step for which the Save to Binary > Budget is selected in the <u>Output</u> <u>Control</u> settings. The SAVE_SPECIFIC_DISCHARGE option is set to no by default. Note that Visual MODFLOW Flex calculates these terms for the velocity outputs so it is not required/redundant.
- THICKSTRT If the THICKSTRT option is set to yes, then cells having a negative ICELLTYPE are confined, and their cell thickness for conductance calculations will be computed as STRT-BOT rather than TOP-BOT. Note that Visual MODFLOW Flex currently only translates ICELLTYPE = 1. The THICKSTRT option is set to no by default.
- VARIABLE_CV If the VARIABLE_CV option is set to yes, then the vertical conductance will be calculated using the saturated thickness and properties of the overlying cell and the thickness and properties of the underlying cell. If the DEWATERED keyword is also set to yes, then the vertical conductance is calculated using only the saturated thickness and properties of the overlying cell if the head in the underlying cell is below its top. If both these options are set to no, then the default condition is to calculate the vertical conductance at the start of the simulation using the initial head and the cell properties. The vertical conductance remains constant for the entire simulation. The VARIABLE_CV is set to no by default.

Grid Data Block

The parameters described below can be specified on a per-layer basis using a collection. To access the desired collection, click in the (Collection) cell and then click the ... button. You can select more than one layer simultaneously using the mouse pointer and the [SHIFT] and [CTRL] keys and define the criteria simultaneously for the selected layer(s).

- **Angle1** is a rotation angle of the hydraulic conductivity tensor in degrees. The angle represents the first of three sequential rotations of the hydraulic conductivity ellipsoid. With the K11 (Kx), K22 (Ky), and K33 (Kz) axes of the ellipsoid initially aligned with the x, y, and z coordinate axes, respectively. ANGLE1 rotates the ellipsoid about its K33 axis (within the x y plane). A positive value represents counter-clockwise rotation when viewed from any point on the positive K33 axis, looking toward the center of the ellipsoid. A value of zero indicates that the K11 axis lies within the x z plane. If ANGLE1 is not specified, default values of zero are assigned to ANGLE1, ANGLE2, and ANGLE3, in which case the K11, K22, and K33 axes are aligned with the x, y, and z axes, respectively.
- **Angle2** is a rotation angle of the hydraulic conductivity tensor in degrees. The angle represents the second of three sequential rotations of the hydraulic conductivity ellipsoid. Following the rotation by ANGLE1 described above, ANGLE2 rotates the ellipsoid about its K22 axis (out of the x y plane). An array can be specified for ANGLE2 only if ANGLE1 is also specified. A positive value of ANGLE2 represents clockwise rotation when viewed from any point on the positive K22 axis, looking toward the center of the ellipsoid. A value of zero indicates that the K11 axis lies within the x y plane. If ANGLE2 is not specified, default values of zero are assigned to ANGLE2 and ANGLE3; connections that are not user-designated as vertical are assumed to be

strictly horizontal (that is, to have no z component to their orientation); and connection lengths are based on horizontal distances.

Angle3 - is a rotation angle of the hydraulic conductivity tensor in degrees. The angle represents the third of three sequential rotations of the hydraulic conductivity ellipsoid. Following the rotations by ANGLE1 and ANGLE2 described above, ANGLE3 rotates the ellipsoid about its K11 axis. An array can be specified for ANGLE3 only if ANGLE1 and ANGLE2 are also specified. An array must be specified for ANGLE3 if ANGLE2 is specified. A positive value of ANGLE3 represents clockwise rotation when viewed from any point on the positive K11 axis, looking toward the center of the ellipsoid. A value of zero indicates that the K22 axis lies within the x - y plane.

STO Settings

The following settings are specific to the storage (STO) package:

~	General		
	Ext	.STO	
	Run	Yes	
	Translate	Yes	
\mathbf{v}	OPTIONS		
	SAVE_FLOWS	Yes	
	SS_CONFINED_ONLY	No	
	TVS6	No	

The storage package is only translated if the Model Run Type is set to Transient in the MODFLOW Settings.

Options

SS_CONFINED_ONLY - If the SS_CONFINED_ONLY option is set to yes, then compressible storage is only calculated for a convertible cell (ICONVERT>0) when the cell is under confined conditions (head greater than or equal to the top of the cell). This option has no effect on cells that are marked as being always confined (ICONVERT= 0). This option is identical to the approach used to calculate storage changes under confined conditions in MODFLOW-2005. Note that Visual MODFLOW Flex currently only translates ICONVERT=1. The SS_CONFINED_ONLY option is set to no by default.

WEL Settings

The following settings are specific to the Well (WEL) package:

×	General		
	Ext	.WEL	
	Run	Yes	
	Translate	Yes	
~	OPTIONS		
	AUTO_FLOW_REDUCE	No	
	AUTO_FLOW_REDUCE_CSV	No	
	AUTO_FLOW_REDUCE_THRESHOLD	0.1	
	BOUNDNAMES	Yes	
	Mover	No	
	PRINT_FLOWS	No	
	PRINT_INPUT	No	
	SAVE_FLOWS	Yes	
	Use as Obs Targets	No	
	Use Time Series	No	

Options

- AUTO_FLOW_REDUCE If the AUTO_FLOW_REDUCE option is set to yes, then the AUTO_FLOW_REDUCE_THRESHOLD value (see below) will be read.By default, AUTO_FLOW_REDUCE is set to no and negative pumping rates are not reduced during a simulation.
- AUTO_FLOW_REDUCE_CSV If both this option and AUTO_FLOW_REDUCE are set to yes, then a new record will be written for each well in the well group for each time step in which the user-requested extraction rate is reduced by the program to a the : .\GWF\{Conceptual Model}.{Well Group}.WEL.csv. AUTO FLOW REDUCE CSV is set to no by default.
- AUTO_FLOW REDUCE_THRESHOLD a value used to define the fraction of the cell thickness used as an interval for smoothly adjusting negative pumping (i.e. withdrawal) rates to 0 in cells with head values less than or equal to the bottom of the cell. Negative pumping rates are adjusted to 0 or a smaller negative value when the head in the cell is equal to or less than the calculated interval above the cell bottom. AUTO_FLOW_REDUCE is set to 0.1 if the specified value is less than or equal to zero. By default, AUTO_FLOW_REDUCE is set to no and negative pumping rates are not reduced during a simulation.

EVT Settings

The following settings are specific to the Evapotranspiration (EVT) package:

~	General	
	Ext	.EVT
	Run	Yes
	Translate	Yes
\mathbf{v}	OPTIONS	
	BOUNDNAMES	Yes
	FIXED_CELL	No
	FORMAT	AsArray
	PRINT_FLOWS	No
	PRINT_INPUT	No
	SAVE_FLOWS	Yes
	Use as Obs Targets	No
	Use Time Series	No

Options

- FIXED_CELL if this option is set to yes, then evapotranspiration will not be reassigned to a cell underlying the cell if that cell is inactive. If this option is set to no, then evapotranspiration will be applied to the uppermost active cell. This option is set to no by default.
- FORMAT there are two methods of inputting evapotranspiration data:
 - o AsArray [default] evapotranspiration data will be written to a layer-based array
 - AsList evapotranspiration data will be written to a list of cells along with the corresponding cell id

RCH Settings

The following settings are specific to the Recharge (RCH) package:

~	General	
	Ext	.RCH
	Run	Yes
	Translate	Yes
\sim	OPTIONS	
	BOUNDNAMES	Yes
	FIXED_CELL	No
	FORMAT	AsArray
	PRINT_FLOWS	No
	PRINT_INPUT	No
	SAVE_FLOWS	Yes
	Use as Obs Targets	No
	Use Time Series	No

Options

• FIXED_CELL - if this option is set to yes, then recharge will not be reassigned to a cell underlying the cell if that cell is inactive. If this option is set to no, then recharge will be applied to the uppermost active cell. This option is set to no by default.

- FORMAT there are two methods of inputting recharge data:
 - o AsArray [default] recharge data will be written to a layer-based array
 - AsList recharge data will be written to a list of cells along with the corresponding cell id

OC Settings

The following settings are specific to the Output Control (OC) package:

✓ General	General		
Ext		.OC	
Run		Yes	
Translate		Yes	
OPTIONS			
BUDGETCSV		No	
OPTIONS/P	OPTIONS/PRINT_FORMAT		
COLUMNS		1	
DIGITS		4	
FORMAT		General	
WIDTH		20	

Options

• **BUDGET_CSV** - if this option is set to yes, then a CSV file containing the budget summary similar to what is printed in the list file will be created during the simulation. A budget summary will be printed for each time step in the simulation. This option is set to no by default.

Options/Print Format

The following options relate to the numerical format of the BUDGET_CSV file (if the option is set to yes):

- Columns: the number of columns for writing data
- Digits: the number of digits to use for writing a number
- Width: the number of characters that will be used to write numbers, including white space
- Format: the number format can be: General [default], Fixed, Exponential, or Scientific

DIS(V) Settings

The following settings are specific to the Discretization (by Vertices) (DIS/V) package:

~	General	
	Ext	.DIS
	Run	Yes
	Translate	Yes
~	OPTIONS	
	NOGRB	No

Options

• **NOGRB** - if this option is set to yes, then MODFLOW-6 will not create a binary grid file. The binary grid file is a common file format for the grid that is used by other modeling codes such as MOD-PATH3DU and certain PEST utilities. This option is set to no by default and a binary grid file will be created.

CHD Settings

The following settings are specific to the specified head (CHD) package:

~	General		
	Ext	.CHD	
	Run	Yes	
	Translate	Yes	
~	OPTIONS		
	BOUNDNAMES	Yes	
	PRINT_FLOWS	No	
	PRINT_INPUT	No	
	SAVE_FLOWS	Yes	
	Use as Obs Targets	No	
	Use Time Series	No	
\mathbf{v}	Misc		
	Duplicate CHD6 Cell Filter	Average	

- Duplicate CHD Cell Filter When working with conceptual models, in some cases
 multiple constant head cells may be assigned to the same cell. When MODFLOW
 formulates the system of equations, it simply adds boundary conditions for all other
 boundary conditions this is usually not a problem as these values still require a head
 solution for that cell; however adding the constant head values together typically does
 not produce the desired result. Therefore, Visual MODFLOW Flex includes an
 optional filter to handle these cases on translation:
 - *Minimum* the minimum specified head value for the current stress period in the cell(s) with multiple values will be assigned
 - Maximum the maximum specified head value for the current stress period in the cell(s) with multiple values will be assigned
 - Average [Default] the arithmetic mean of specified head values for the current stress period in the cell(s) with multiple values will be assigned
 - Sum specified head values values for the current stress period in the cell(s) with multiple values will be added.

SIM Settings

The following settings are specific to the specified head MODFLOW Simulation file (MFSIM.NAM):

\sim	General	
	Ext	.NAM
	Run	Yes
	Translate	Yes
\sim	OPTIONS	
	CONTINUE	No
	MAXERRORS	10
	MEMORY_PRINT_OPTION	None
	NOCHECK	No

- **CONTINUE** if this option is set to yes, then MODFLOW-6 will continue with the remaining solution groups if one or more solutions do not converge. For example, if a transport model does not converge, then the flow model may continue through the rest of the simulation. By default, this option is set to no and the simulation will stop if any model in the simulation does not converge within the specified number of iterations.
- MAXERRORS maximum number of errors that will be stored and printed.
- **MEMORY_PRINT_OPTION** is a flag that controls printing of detailed memory manager usage to the end of the simulation list file.
 - o NONE [default] means do not print detailed information.
 - o SUMMARY means print only the total memory for each simulation component.
 - o ALL means print information for each variable stored in the memory manager.
- NOCHECK if this option is set to yes, then MODFLOW-6 will not perform checks on the model input files. Checks are performed by default.

NAM Settings

The following settings are specific to the Flow Model Name (NAM) file:

~	General	
	Ext	.NAM
	Run	Yes
	Translate	Yes
\mathbf{v}	OPTIONS	
	NEWTON	Yes
	PRINT_FLOWS	Yes
	PRINT_INPUT	No
	SAVE_FLOWS	Yes
	UNDER_RELAXATION	Yes

- **NEWTON** if this option is set to yes, then the simulation will use the Newton-Raphson formulation for groundwater flows between connected, convertible groundwater cells and stress packages that support calculation of Newton-Raphson terms for groundwater exchanges. Cells will not dry when this option is used. By default, the Newton-Raphson formulation is applied.
- UNDER-RELAXATION if this option is set to yes, the groundwater head in a cell will be underrelaxed when water levels fall below the bottom of the model below any given cell. By default this option is set to yes, and the Newton-Raphson UNDER_RELAXATION is applied. This option is ignored if the NEWTON option is set to no.

10.10.3 MODFLOW-6 Transport

This chapter describes the features, functionality, and options in the Translation section of the Visual MODFLOW Flex interface when using MODFLOW-6 to perform the groundwater transport (GWT) simulation.



If you are not familiar with MODFLOW-6 and how it has been implemented in Visual MODFLOW Flex, it is <u>strongly</u> <u>recommended</u> that you familiarize yourself with the MODFLOW-6 framework and input file structure, particularly if you intend to use some of the advanced features available in MODFLOW-6 and/or you wish to work with the input files directly.

At a minimum, please read <u>Introduction to MODFLOW-6</u> and the subtopics in the present section.

MODFLOW-6 Groundwater Transport Model Settings:

- Settings MODFLOW-6 Transport
- Solver Settings
- Initial Concentrations
- Output Control
- Advanced Settings

10.10.3.1 MODFLOW-6 Transport Settings

The following general settings are available for the MODFLOW-6 transport engine:

Porosity Options

The Porosity options are used to select which porosity measurement to use for the transport solution.

- For advection-dominated transport, the best choice is to apply the "Effective" porosity option, then diffusion into and out of dead-end pore spaces can be considered negligible.
- For diffusion-dominated transport, the best choice is to select the "Total" porosity option to account for mass transfer to and from dead-end pore spaces.

10.10.3.2 Solver Settings

Solvers in MODFLOW-6 are handled through the iterative model solution (IMS) package which is used to solve flow and/or transport simulations. The IMS package uses a linear and non-linear methods to solve the simultaneous equations produced by the model(s) as described below:

ettings Translation Log nam T	DIS IMS DIS IC OC NPF	CHD CHD(2) RIV WEL STO nam(2)
General Settings MODFLOW-6 Settings Solvers	General Selected Solver	Iterative Matrix Solver (IMS)
Initial Heads Output Control Advanced Settings General General Initial Concentrations Output Control	Options PrintOption Complexity CsvOuterOutput CsvInnerOutput NoPtc AtsOuterMaximumFraction Linear	None Simple False False First 0.25
⊕. Advanced Settings	InnerMaximum InnerDVClose InnerRClose LinearAcceleration RelaxationFactor PreconditionerLevels PreconditionerDropTolerance NumberOrthogonalizations ScalingMethod	100 1E-06 BICGStab 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
	ReorderingMethod Nonlinear OuterDVClose OuterMaximum UnderRelaxationGamma UnderRelaxationGamma UnderRelaxationTheta UnderRelaxationTheta UnderRelaxationMomentum BacktrackingNumber BacktrackingTolerance BacktrackingReductionFactor BacktrackingResidualLimit	None 0.01 100 None 0.2 0.7 0.1 0.001 10 10000 0.2 100
, n n s	PrintOption A flag that controls printing of convergence informeans print nothing. SUMMARY means print onl residual reduction summaries. ALL means print im solution listing file and model specific linear matrix listing file in addition to SUMMARY information. N	r the total number of iterations and nonlinear ear matrix solver convergence information to the solver convergence information to each model

General Solution Options

The following settings are optional in the IMS package:

- PrintOption: An optional keyword setting that determines the print level of the solver in the listing file:
 - Summary means print only the total number of iterations and nonlinear residual reduction summaries.
 - All means print linear matrix solver convergence information to the solution listing file and model specific linear matrix solver convergence information to each model listing file in addition to Summary information.
 - o None means that no solver information will be printed. This is the default option.
- Complexity: is an optional keyword that defines default non-linear and linear solver parameters.

- Simple indicates that default solver input values will be defined that work well for nearly linear models. This option is generally suitable for models that do not include nonlinear stress packages and models that are either confined or consist of a single unconfined layer that is thick enough to contain the water table within a single layer.
- Moderate: indicates that default solver input values will be defined that work well for moderately nonlinear models. This option is generally suited for models that include nonlinear stress packages and models that consist of one or more unconfined layers. The *Moderate* option should be used when the *Simple* option does not result in successful convergence.
- Complex: indicates that default solver input values will be defined that work well for highly nonlinear models. This option is generally suited for models that include nonlinear stress packages and models that consist of one or more unconfined layers representing complex geology and surface-water/groundwater interaction. The complex option should be used when the moderate option does not result in successful convergence.
- Custom: indicates that custom values will be defined for the linear and non-linear solvers.

If the Simple, Moderate, or Complex options are selected, then only the items in the linear and non-linear solver sections below marked with * will be translated. All other options will use the defaults below:

SETTINGS	COMPLEXITY				
SETTINGS	SIMPLE	MODERATE	COMPLEX		
NON-LINEAR SOLVER SE	TTINGS				
OUTER_DVCLOSE *	0.001	0.01	0.1		
OUTER_MAXIMUM *	25	50	100		
UNDER_RELAXATION	NONE	DBD	DBD		
UNDER_RELAXATION_TH ETA	1	0.9	0.8		
UNDER_RELAXATION_KA PPA	0	0.0001	0.0001		
UNDER_RELAXATION_G AMMA	0	0	0		
UNDER_RELAXATION_M OMENTUM	0	0	0		
BACKTRACKING_NUMBE R	0	0	20		
BACKTRACKING_TOLER ANCE	0	0	1.05		

BACKTRACKING_REDUC TION_FACTOR	0	0	0.1
BACKTRACKING_RESIDU AL_LIMIT	0	0	0.002
LINEAR SOLVER SETTING	S		
INNER_MAXIMUM *	50	100	500
INNER_DVCLOSE *	0.001	0.01	0.1
INNER_RCLOSE *	0.1	0.1	0.1
RCLOSE_OPTION	infinity-norm	infinity-norm	infinity-norm
LINEAR_ACCELERATION	CG	BICGSTAB	BICGSTAB
RELAXATION_FACTOR	0	0.97	0
PRECONDITIONER_LEVE LS	0	0	5
PRECONDITIONER_DRO P_TOLERANCE	0	0	0.0001
NUMBER_ORTHOGONALI ZATIONS	0	0	2
SCALING_METHOD	NONE	NONE	NONE
REORDERING_METHOD	NONE	NONE	NONE

- **CsvOuterOutput**: if this option is set to yes, then outer iteration convergence information will be written to a comma separated values file in the GWF subfolder. This option is off by default. Information written to this file includes maximum dependent-variable (for example, head or concentration) change convergence information at the end of each outer iteration for each time step.
- **CsvInnerOutput**: if this option is set to yes, then inner iteration convergence information will be written to a comma separated values file in the GWF subfolder. This option is off by default. Information written to this file includes maximum dependent-variable (for example, head or concentration) change and maximum residual convergence information for the solution and each model (if the solution includes more than one model) and linear acceleration information for each inner iteration.
- NoPTC: is a settings that is used to control the pseudo-transient continuation (PTC) options for steady state periods for models using the Newton-Raphson formulation (which is controlled by in NAM file <u>settings</u>):
 - o None: PTC will not be used in solution
 - o First. PTC will be activated for the first stress period
 - o All: PTC will be deactivated for all stress periods

For many problems, PTC can significantly improve convergence behavior for steadystate simulations, and for this reason it is active by default. In some cases; however, PTC can worsen the convergence behavior, especially when the initial conditions are similar to the solution. When the initial conditions are similar to (or exactly the same as) the solution and convergence is slow, then the NO_PTC FIRST option should be used to deactivate PTC for the first stress period. The NO_PTC ALL option should also be used in order to compare convergence behavior with other MODFLOW versions, as PTC is only available in MODFLOW 6.

• AtsOuterMaximumFraction: real value defining the fraction of the maximum allowable outer iterations used with the Adaptive Time Step (ATS) capability if it is active. If this value is set to zero by the user, then this solution will have no effect on ATS behavior. This value must be greater than or equal to zero and less than or equal to 0.5 or the program will terminate with an error. If it is not specified by the user, then it is assigned a default value of one third. When the number of outer iterations for this solution is less than the product of this value and the maximum allowable outer iterations, then ATS will increase the time step length by a factor of DTADJ in the ATS input file. When the number of outer iterations for this solution is greater than the maximum allowable outer iterations, then ATS (if active) will decrease the time step length by a factor of 1 / DTADJ.

Non-Linear Solver Options

The following settings are available for the Non-linear solver:

- OUTER_DVCLOSE: real value defining the dependent-variable (for example, head or concentration) change criterion for convergence of the outer (nonlinear) iterations, in units of the dependent-variable (for example, length for head or mass per length cubed for concentrations). When the maximum absolute value of the dependent-variable change at all nodes during an iteration is less than or equal to OUTER_DVCLOSE, iteration stops.
- **OUTER_MAXIMUM**: integer value defining the maximum number of outer (nonlinear) iterations. For a linear problem OUTER_MAXIMUM should be 1.
- UNDER_RELAXATION: an optional keyword that defines the nonlinear underrelaxation schemes used. Under-relaxation is also known as dampening, and is used to reduce the size of the calculated dependent variable before proceeding to the next outer iteration. Under-relaxation can be an effective tool for highly nonlinear models when there are large and often counteracting changes in the calculated dependent variable between successive outer iterations. By default under-relaxation is not used.
 - o NONE [Default] under-relaxation is not used
 - SIMPLE Simple under-relaxation scheme with a fixed relaxation factor (under relaxation gamma (see below)) is used.
 - o COOLEY Cooley under-relaxation scheme is used.
 - o DBD delta-bar-delta (DBD) under-relaxation is used.

Note that the under-relaxation schemes are often used in conjunction with problems that use the Newton-Raphson formulation (which is controlled by in NAM file <u>settings</u>); however, experience has indicated that they also work well for non-Newton problems, such as those with the wet/dry options of MODFLOW 6.

- UNDER_RELAXATION_GAMMA: a real value defining either the relaxation factor for the simple complexity scheme or the history or memory term factor of the Cooley and delta-bar-delta algorithms. For the simple scheme, a value of one indicates that there is no under-relaxation and the full head (or concentration) change is applied. This value can be gradually reduced from one as a way to improve convergence; for well behaved problems, using a value less than one can increase the number of outer iterations required for convergence and needlessly increase run times. Under relaxation gamma must be greater than zero for the simple scheme or the program will terminate with an error. For the Cooley and delta-bar-delta schemes, Under relaxation gamma is a memory term that can range between zero and one. When Under relaxation gamma is zero, only the most recent history (previous iteration value) is maintained. As Under relaxation gamma is increased, past history of iteration changes has greater influence on the memory term. The memory term is maintained as an exponential average of past changes. Retaining some past history can overcome granular behavior in the calculated function surface and therefore helps to overcome cyclic patterns of non-convergence. The value usually ranges from 0.1 to 0.3; a value of 0.2 works well for most problems. Under relaxation gamma is only used in the simulation if Under relaxation is not None.
- UNDER_RELAXATION_THETA: a real value defining the reduction factor for the learning rate (underrelaxation term) of the delta-bar-delta algorithm. The value of *under relaxation theta* is between zero and one. If the change in the dependent-variable (for example, head or concentration) is of opposite sign to that of the previous iteration, the under-relaxation term is reduced by a factor of *under relaxation theta*. The value usually ranges from 0.3 to 0.9; a value of 0.7 works well for most problems. *Under relaxation theta* is only used in the simulation if *under relaxation* is DBD.
- UNDER_RELAXATION_KAPPA: a real value defining the increment for the learning rate (under-relaxation term) of the delta-bar-delta algorithm. The value of *under relaxation kappa* is between zero and one. If the change in the dependent-variable (for example, head or concentration) is of the same sign to that of the previous iteration, the under-relaxation term is increased by an increment of *under relaxation kappa*. The value usually ranges from 0.03 to 0.3; a value of 0.1 works well for most problems. *Under relaxation kappa* is only used in the simulation if *under relaxation* is DBD.
- UNDER_RELAXATION_MOMENTUM: a real value defining the fraction of past history changes that is added as a momentum term to the step change for a nonlinear iteration. The value of *under relaxation momentum* is between zero and one. A large momentum term should only be used when small learning rates are expected. Small amounts of the momentum term help convergence. The value usually ranges from 0.0001 to 0.1; a value of 0.001 works well for most problems. *Under relaxation momentum* is only used in the simulation if *under relaxation* is DBD.
- **BACKTRACKING_NUMBER**: an integer value defining the maximum number of backtracking iterations allowed for residual reduction computations. If *backtracking*

number = 0 then the backtracking iterations are omitted. The value usually ranges from 2 to 20; a value of 10 works well for most problems.

- **BACKTRACKING_TOLERANCE**: a real value defining the tolerance for residual change that is allowed for residual reduction computations. The *backtracking tolerance* value should not be less than one to avoid getting stuck in local minima. A large value serves to check for extreme residual increases, while a low value serves to control step size more severely. The value usually ranges from 1.0 to 106; a value of 104 works well for most problems but lower values like 1.1 may be required for harder problems. *Backtracking tolerance* is only used in the simulation if *backtracking number* is greater than zero.
- **BACKTRACKING_REDUCTION_FACTOR**: real value defining the reduction in step size used for residual reduction computations. The value of is between zero and one. The value usually ranges from 0.1 to 0.3; a value of 0.2 works well for most problems. *Backtracking reduction factor* is only used in the simulation if *backtracking number* is greater than zero.
- **BACKTRACKING_RESIDUAL_LIMIT**: a real value defining the limit to which the residual is reduced with backtracking. If the residual is smaller than *backtracking residual limit*, then further backtracking is not performed. A value of 100 is suitable for large problems and residual reduction to smaller values may only slow down computations. *Backtracking residual limit* is used in the simulation if *backtracking number* is greater than zero.

Linear Solver Options

The following settings are available for the Linear solver:

- **INNER_MAXIMUM**: an integer value defining the maximum number of inner (linear) iterations. The number typically depends on the characteristics of the matrix solution scheme being used. For nonlinear problems, *inner maximum* usually ranges from 60 to 600; a value of 100 will be sufficient for most linear problems.
- INNER_DVCLOSE: a real value defining the dependent-variable (for example, head or concentration) change criterion for convergence of the inner (linear) iterations, in units of the dependent-variable (for example, length for head or mass per length cubed for concentration). When the maximum absolute value of the dependent-variable change at all nodes during an iteration is less than or equal to *inner dvclose*, the matrix solver assumes convergence. Commonly, *inner_dvclose* is set equal to or an order of magnitude less than the *outer_dvclose* value specified for the non-linear block.
- **INNER_RCLOSE**: a real value that defines the flow residual tolerance for convergence of the IMS linear solver and specific flow residual criteria used. This value represents the maximum allowable residual at any single node. Value is in units of length cubed per time, and must be consistent with MODFLOW-6 length and time units. Usually a value of 0.1 is sufficient for the flow-residual criteria when meters and seconds are the defined MODFLOW-6 length and time.

- ∆h ≤
 - **RCLOSE_OPTION**: an optional keyword that defines the specific flow residual criterion used.
 - STRICT: an optional keyword that is used to specify that *inner rclose* represents a infinity-Norm (absolute convergence criteria) and that the dependent-variable (for example, head or concentration) and flow convergence criteria must be met on the first inner iteration (this criteria is equivalent to the criteria used by the MODFLOW-2005 PCG package (Hill, <u>1990</u>)).
 - L2NORM_RCLOSE: an optional keyword that is used to specify that *inner rclose* represents a L-2 Norm closure criteria instead of a infinity-Norm (absolute convergence criteria). When *L2norm rclose* is specified, a reasonable initial *inner rclose* value is 0.1 times the number of active cells when meters and seconds are the defined MODFLOW-6 length and time.
 - RELATIVE_RCLOSE: an optional keyword that is used to specify that *inner rclose* represents a relative L-2 Norm reduction closure criteria instead of a infinity-Norm (absolute convergence criteria). When *relative rclose* is specified, a reasonable initial *inner rclose* value is 1.0×10⁻⁴ and convergence is achieved for a given inner (linear) iteration when *inner dvclose* and the current L-2 Norm is ≤ the product of the *relative_rclose* and the initial L-2 Norm for the current inner (linear) iteration. If *rclose option* is not specified, an absolute residual (infinity-norm) criterion is used.
 - LINEAR ACCELERATION: a keyword that defines the linear acceleration method used by the default IMS linear solvers.
 - o CG preconditioned conjugate gradient method.
 - o BICGSTAB preconditioned bi-conjugate gradient stabilized method.
 - **RELAXATION_FACTOR**: an optional real value that defines the relaxation factor used by the incomplete LU factorization preconditioners (MILU(0) and MILUT). *Relaxation_factor* is unitless and should be greater than or equal to 0.0 and less than or equal to 1.0. *Relaxation factor* values of about 1.0 are commonly used, and experience suggests that convergence can be optimized in some cases with relax values of 0.97. A *Relaxation factor* value of 0.0 will result in either ILU(0) or ILUT preconditioning (depending on the value specified for *preconditioner levels* and/or *preconditioner drop tolerance*). By default, *relaxation factor* is zero.
 - **PRECONDITIONER_LEVELS**: an optional integer value defining the level of fill for ILU decomposition used in the ILUT and MILUT preconditioners. Higher levels of fill provide more robustness but also require more memory. For optimal performance, it is suggested that a large level of fill be applied (7 or 8) with use of a drop tolerance. Specification of a *preconditioner levels* value greater than zero results in use of the ILUT preconditioner. By default, the number of *preconditioner levels* is zero and the zero-fill incomplete LU factorization preconditioners (ILU(0) and MILU(0)) are used.
 - PRECONDITIONER_DROP_TOLERANCE: a real value that defines the drop tolerance used to drop preconditioner terms based on the magnitude of matrix entries in the ILUT and MILUT preconditioners. A value of 10⁻⁴ works well for most problems. By default, the *preconditioner drop tolerance* is zero and the zero-fill incomplete LU factorization preconditioners (ILU(0) and MILU(0)) are used.

- NUMBER_ORTHOGONALIZATIONS: an integer value defining the interval used to explicitly recalculate the residual of the flow equation using the solver coefficient matrix, the latest dependent/variable (for example, head or concentration) estimates, and the right hand side. For problems that benefit from explicit recalculation of the residual, a number between 4 and 10 is appropriate. By default, the *number of orthogonalizations* is zero.
- SCALING_METHOD: an optional keyword that defines the matrix scaling approach used. By default, matrix scaling is not applied.
 - o NONE [Default] no matrix scaling applied.
 - DIAGONAL symmetric matrix scaling using the POLCG preconditioner scaling method in Hill (<u>1990</u>).
 - o L2NORM symmetric matrix scaling using the L-2 Norm.
- **REODERING_METHOD**: an optional keyword that defines the matrix reordering approach used. By default, matrix reordering is not applied.
 - o NONE [Default] original ordering.
 - o RCM reverse Cuthill McKee ordering.
 - *MD* minimum degree ordering.

10.10.3.3 Initial Concentrations

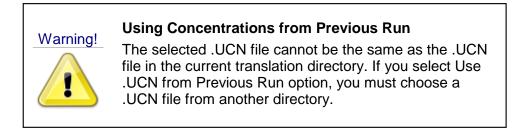
In Visual MODFLOW Flex, the Initial Concentrations are typically defined at the <u>Define</u> <u>Properties</u> step in the workflow. For more details, please see the section on setting <u>Initial</u> <u>Concentrations</u>. However, in some cases, it may be preferable to use alternate values from a previous model run. As such, the initial concentrations that will be translated for the simulation can be specified by species using the table shown below:

Settings Translation Log nam TDIS IMS DIS	IC OC	NPF CHD CHD	(2) RIV WEL STO nam(2)				
- General	ld	Species Name	Option	FilePath	Browse		
	001	Conc001	SPECIFIED		Browse		
Solves Vital Concentrations Output Control D Advanced Settings							

- Id: The index of the species in the transport simulation as defined in the Modeling Objectives step.
- Species Name: The name of the species
- Option:
 - Specified [Default]: will use the values that are defined for "Initial Concentrations" at the Define Properties step.

 Previous_Run: requires you to select a .UCN file from a previous transport Run and specify the Time step to be used. The .UCN file must be based on the same grid type and number of cells in each applicable dimension (i.e. layer, row, and columns for a structured grid, and same number of layers and cells per layer for an unstructured grid).

Select previous UCN file		_		×
Time step			Brows	e
	01	K	Cance	əl



10.10.3.4 Output Control

The Output Control options set the information and frequency of information written and saved to the MODFLOW-6 output files (see following figure).

Define Modeling Objectives Define Properties Define Boundary Conditions	Settings Translation Log							
Select Next Step	General	🖋 Every Nth s	tep 1 🔳	Concentration	n (Print to 🗸 👻			
Define Zone Budget Zones	MODFLOW-6				Save to bir	arv	Print to .L	ST
Define Particles	Settings	End Time	Stress Period	True Cher	Concentration		Concentration	Dudaat
Select Run Type	Solvers		Stress Period	Time Step	Concentration	Budget	Concentration	Budget
Single Run	Initial Heads	0.13	1	1				
Translate	Output Control	0.28	1	2				
Run	Advanced Settings	0.44	1	3				
View Results	MODFLOW-6 Transport-Specific	0.61	1	4				
View Charts	General	0.81	1	5				
View Maps	Solvers	1.022	1	6				
	Initial Concentrations	1.26	1	7				
	Output Control Advanced Settings	1.51	1	8				
		1.8	1	9				
		2.11	1	10	\checkmark	\checkmark		\checkmark
		2.45	1	11				
		2.83	1	12				
		3.25	1	13				
		3.71	1	14				
		4.21	1	15				
		4.76	1	16				
		5.37	1	17	Π		Π	Π
		6.039	1	18	Π			
		6.78	1	19			Π	
		7.59	1	20				
		8.48	1	21	Π		Π	
		9.46	1	22		Π		
		10.53	1	23			Π	
		11.72	1	24				
		13.025	1	25				П

By default, each MODFLOW-6 groundwater transport model simulation will produce several output files as described below. The Output Control settings allow you to specify the stress period(s)/time step(s) for which model results of interest will be written to these output files. The Output Control Settings are provided in a tabular format:

- Schedule:
 - End Time: the elapsed simulation time corresponding to the end of the specified stress period and time step
 - o Stress Period: the stress period in the schedule
 - o Time Step: the time step within the stress period
- Save to Binary:
 - Concentration: simulated heads will be written to the binary heads file (. \GWF\modelname.HDS) for active cells in the grid for selected End Times (Stress Period/Time Step)
 - Budget: mass budget terms will be written to the binary budget file (. \GWF\modelname.BGT) for active cells and boundary conditions in the grid for selected End Times (Stress Period/Time Step).

Please Note: for cell-by-cell values to be added to the budget file, the SAVE_FLOWS option must be enabled (set to "Yes") in the Advanced Settings for the NAM package. Similarly, for cell-to-boundary condition values to be added to the budget file, the SAVE_FLOWS option must be enabled in the Advanced Settings for each desired boundary condition (e.g. the SSM, CNC, and SRC packages). In Visual MODFLOW Flex, the SAVE_FLOWS option is enabled by default for all supported packages including the NAM file and supported boundary conditions.

• **Print to LST:** information will be written to the listing file (. \GWT\S###\modelname.LST), where S### is the index of each species:

- Concentration: simulated concentrations will be written to the listing file for active cells in the grid for selected End Times (Stress Period/Time Step). Note that this option should be used sparingly, typically for model troubleshooting, particularly as this format can lead to overly large output files that are less efficient to work with than the binary file or related files that can be exported from Visual MODFLOW Flex.
- Budget: net flow budget terms, expressed at a package level, for boundary conditions and internal storage will be written to the listing file for selected End Times (Stress Period/Time Step)

Please Note: for cell-by-cell values to be added to the listing file, the PRINT_FLOWS option must be enabled (set to "Yes") in the Advanced Settings for the NAM package. Similarly, for cell-to-boundary condition values to be added to the budget file, the PRINT_FLOWS option must be enabled in the Advanced Settings for each desired boundary condition. In Visual MODFLOW Flex, the PRINT_FLOWS option is enabled by default for all supported packages including the NAM file and supported boundary conditions.

Saving Output Every Nth Time Step

For simulations with many stress periods and time steps, it can be very tedious to manually select the desired output time step intervals. The row of fields underneath the Output Control table are used to specify regular time step intervals for saving files during Each N-th step in each stress period. The first text box is where the N value is entered. To apply this value to the column, click the underlying checkbox.

If a subsequent engine is included in the run formation (e.g. ZoneBudget) with the MODFLOW simulation, Visual MODFLOW Flex will save the flow terms for all time steps by default.

10.10.3.5 Advanced Settings

Advanced translation settings are available for transport simulations to enable more advanced control of translation and package settings. <u>General</u> and <u>common</u> settings are described in the section on the advanced settings for MODFLOW-6 groundwater flow (GWF) models, while package-specific settings are described below.

MODFLOW-6 - Transport Packages

Package-specific settings for MODFLOW-6 flow model packages are described below:

ADV Settings

The following settings are specific to the Advection (ADV) package:

✓ General		
Ext	.ADV	
Run	Yes	
Scheme	Upstream	
Translate	Yes	

- Scheme This setting allows you to select the solution technique for the transport:
 - o Upstream [Default]: upstream finite difference
 - o Central: central finite difference
 - o TVD: Higher-order Total Variation Diminishing method

These methods are described in more detail, here and here.

CNC Settings

The following settings are specific to the Constant Concentration (CNC) package:

~	General	
	Ext	.CNC
	Run	Yes
	Translate	Yes
\mathbf{v}	OPTIONS	
	BOUNDNAMES	Yes
	PRINT_FLOWS	No
	PRINT_INPUT	No
	SAVE_FLOWS	Yes
	Use Time Series	No
\mathbf{v}	Misc	
	Duplicate CNC6 Cell Filter	Average
	Duplicate CNC6 Cell Filter	Average

- **Duplicate CNC6 Cell Filter** When working with conceptual models, in some cases multiple constant concentration cells may be assigned to the same cell. When MODFLOW formulates the system of equations, it simply adds boundary conditions for all other boundary conditions this is usually not a problem as these values still require a concentration solution for that cell; however adding the constant concentration values together typically does not produce the desired result. Therefore, Visual MODFLOW Flex includes an optional filter to handle these cases on translation:
 - *Minimum* the minimum specified concentration value for the current stress period in the cell(s) with multiple values will be assigned
 - Maximum the maximum specified concentration value for the current stress period in the cell(s) with multiple values will be assigned
 - Average [Default] the arithmetic mean of specified concentration values for the current stress period in the cell(s) with multiple values will be assigned
 - Sum specified concentration values values for the current stress period in the cell(s) with multiple values will be added.

DSP Settings

The following settings are specific to the Dispersion (DSP) package and control how the <u>Dispersion</u> properties in the Define Properties workflow step will be translated:

~	General	
	Ext	.DSP
	Run	Yes
	Translate	Yes
~	OPTIONS	
	ALH - Longitudinal dispersivity in horizontal direction	No
	ALV - Longitudinal dispersivity in vertical direction	No
	ATH1 - Transverse dispersivity in horizontal direction	No
	ATH2 - Transverse dispersivity in horizontal direction	No
	ATV - Transverse dispersivity when flow is in vertical direction	No
	Mechanical Dispersion	No
	Molecular Diffusion	No
	XT3D	None

- ALH: a <u>read-only</u> setting for translating longitudinal dispersivity in the horizontal direction. If flow is strictly horizontal, then this is the longitudinal dispersivity that will be used. If flow is not strictly horizontal or strictly vertical, then the longitudinal dispersivity is a function of both ALH and ALV. If mechanical dispersion is included in the simulation (i.e. the Mechanical Dispersion setting is set to yes) then this settings is set to yes, otherwise, it is set to no.
- ALV: a setting for translating longitudinal dispersivity in the vertical direction. If flow is strictly vertical, then this is the longitudinal dispersivity that will be used. If flow is not strictly vertical, then the longitudinal dispersivity is a function of both ALH and ALV. If this option is set to no and mechanical dispersion is represented, then the ALV values in the dispersion array is not translated and assumed to equal ALH by MODFLOW-6.
- ATH1: a <u>read-only</u> setting for translating the transverse dispersivity in horizontal direction. This is the transverse dispersivity value for the second ellipsoid axis. If flow is strictly horizontal and directed in the x direction (along a row for a regular grid), then this value controls spreading in the y-direction. If mechanical dispersion is included in the simulation (i.e. the Mechanical Dispersion setting is set to yes) then this settings is set to yes, otherwise, it is set to no.
- ATH2: a setting for translating the transverse dispersivity in horizontal direction. This is the transverse dispersivity value for the third ellipsoid axis. If flow is strictly horizontal and directed in the x direction (along a row for a regular grid), then this value controls spreading in the z-direction. If this option is set to no and mechanical dispersion is represented, then this array is not translated and assumed to equal ATH1 by MODFLOW-6.
- **ATV**: a setting for translating the transverse dispersivity when flow is in vertical direction. If flow is strictly vertical and directed in the z-direction, then this value controls spreading in the x and y directions. If this option is set to no and mechanical dispersion is represented, then this array is not translated and assumed to equal ATH2 (or ATH1) by MODFLOW-6.

- **Mechanical Dispersion**: a setting for translating the dispersivity terms (ALH, ALV, ATH1, ATH2, ATV). If set to yes, then ALH and ATH1 will values will be translated and the other dispersivity terms (ALV, ATH2, and ATV) will be translated based on their settings; otherwise, none of these terms will be included and mechanical dispersion terms will be omitted from the solution.
- **Molecular Diffusion**: a setting for translating the diffusion term. If set to yes, then the molecular diffusion term will be included in the simulation.
- **XT3D**: a setting for (de)activating the XT3D method and has the following options:
 - None [Default]: the XT3D formulation will not be used in the solution. This method is generally faster and less accurate. This option may provide a fast and accurate solution under some circumstances, such as when flow aligns with the model grid, there is no mechanical dispersion, or when the longitudinal and transverse dispersivities are equal. This option may also be used to assess the computational demand of the XT3D approach by noting the run time differences with and without this option on.
 - *RHS*: the XT3D formulation will only add dispersion terms to the right-hand side terms in the system of equations for the transport solution. This option uses less memory, but may require more iterations than the full XT3D formulation available by using the Coefficients option.
 - Coefficients: the full XT3D formulation will used and dispersion terms will be added to the coefficient matrix in the system of equations for the transport solution. This option uses the most memory and may be computationally expensive; however, this option may be required to accurately represent dispersion.

FMI Settings

The following settings are specific to the Flow Model Interface (FMI) package and control whether and how the Groundwater Flow (GWF) and Groundwater Transport (GWT) models will be linked:

	a				
\sim	General				
	Ext	.FMI			
	Run	Yes			
	Translate	Yes			
\sim	OPTIONS				
	Exchange	Linked			
	Flow Imbalance Correction	No			
	Save Flows	No			

- Exchange: TBD
- Flow Imbalance Correction: TBD
- Save Flows: TBD

Please Note: the FMI package and GWT6 (Exchange) package are mutually exclusive.

IMST Settings

The following settings are specific to the Iterative Model Solution (IMS) package for Transport models (IMST):

~	General	
	Ext	.IMST
	Run	Yes
	Translate	Yes
	UseSpeciesSpecificClosures	No
~	Species	
	ClosureCriteria	(Collection)

- UseSpeciesSpecificClosures: is a setting that controls whether or not the Species-Specific ClosureCriteria (see below) will be used. This option is set to no by default.
- ClosureCriteria: Is a collection of species-specific settings that allows you to set independent solver <u>closure criteria</u> (i.e. INNER_DVCLOSE, INNER_RCLOSE, OUTER_DVCLOSE) for each species. This may be useful if the concentrations of the species are expected to vary over several orders of magnitude. To access the desired collection, click in the (Collection) cell and then click the ... button. You can select more than one layer simultaneously using the mouse pointer and the [SHIFT] and [CTRL] keys and define the criteria simultaneously for the selected layer(s).

IMSSpeciesType Collection Editor			?	\times
Members: 0 PCE 1 TCE 2 DCE 3 VC 4 ETH 5 CI-	↑ ↓	PCE properties: Misc INNER_DVCLOSE INNER_RCLOSE OUTER_DVCLOSE Species	1E-06 1E-06 0.01 001	
Add Remove		ОК	Cance	

IST Settings

The settings described below are specific to the Immobile Storage and Transfer (IST) package and will only be used if the <u>Transport Modeling Objectives</u> include either, the Dual Domain With Complex Sorption, the Triple Domain with Complex Sorption, or the Quadruple Domain with Complex Sorption Retardation Models.

~	General		
	Ext	.IST	
	Run	Yes	
	Translate	Yes	
~	OPTIONS		
	BUDGET FILEOUT	conceptual-model.bgt	
	BUDGETCSV FILEOUT	conceptual-model.bgt.csv	
	CIM FILEOUT	conceptual-model.cim.ucn	
	SAVE_FLOWS	Yes	
~	Species		
	Immobile1	(Collection)	
	Immobile2	(Collection)	
	Immobile3	(Collection)	

The following settings are available for the active immobile domain(s) in the Immobile Storage and Transfer package:

- Immobile1: is a collection of settings for the first immobile domain
- Immobile2: is a collection of settings for the second immobile domain
- Immobile3: is a collection of settings for the third immobile domain

Each one of these collections of settings can be accessed by clicking in the desired (Collection) cell and clicking the ... button, which will open the IST Immobile Domain Settings window with the following settings described below. You can select more than one layer simultaneously using the mouse pointer and the [SHIFT] and [CTRL] keys and define the criteria simultaneously for the selected layer(s).

DomainTypeWrapper Collection Edito	or			?	×
Members: 0 PCE 1 TCE 2 DCE 3 VC 4 ETH 5 CI-	↑ ↓	Multi-Select Prope		icReact tion	ions
<u>A</u> dd <u>R</u> emove					
			ОК	Cano	el

- **IREACT**: an option to specify the reaction model for the selected species in the selected immobile domain
 - NoKinetic Reaction: No kinetic reactions will be included in the simulation for the selected species
 - FirstOrderIrreversibleDecay: the selected species will be simulated for the selected species
 - *ZerothOrderIrreversibleDecay*: the selected species will be simulated for the selected species
- **ISOTHM**: an option to specify the retardation model for the selected species in the selected immobile domain
 - NoSorption: No sorption reactions will be included in the simulation for the selected species
 - o Linear: the linear sorption isotherm will be simulated for the selected species

MST Settings

The settings described below are specific to the Mobile Storage and Transfer (MST) package and will only be used if the <u>Transport Modeling Objectives</u> include either, the Dual Domain With Complex Sorption, the Triple Domain with Complex Sorption, or the Quadruple Domain with Complex Sorption Retardation Models.

~	General	
	Ext	.MST
	Run	Yes
	Translate	Yes
~	OPTIONS	
	SAVE_FLOWS	Yes
~	Species	
	Mobile	(Collection)

The following settings are available for the active immobile domain(s) in the Immobile Storage and Transfer package:

• **Mobile**: is a collection of settings for the mobile domain. The mobile collection of settings can be accessed by clicking in the (Collection) cell and clicking the ... button, which will open the MST Mobile Domain Settings window with the following settings described below. You can select more than one species simultaneously using the mouse pointer and the [SHIFT] and [CTRL] keys and define the criteria simultaneously for the selected species(s).

DomainTypeWrapper Collection Edito	or			?	×
Members:	↑ ↓	Multi-Select Properties	No Kinet No Sorpt		ons
		0)K	Cance	el:

- **IREACT**: an option to specify the reaction model for the selected species in the selected immobile domain
- NoKinetic Reaction: No kinetic reactions will be included in the simulation for the selected species
- *FirstOrderIrreversibleDecay*: the selected species will be simulated for the selected species

- *ZerothOrderIrreversibleDecay*: the selected species will be simulated for the selected species
 - **ISOTHM**: an option to specify the retardation model for the selected species in the selected immobile domain
- NoSorption: No sorption reactions will be included in the simulation for the selected species
- o Linear: the linear sorption isotherm will be simulated for the selected species
- o Freundlich: the Freundlich isotherm will be simulated for the selected species
- o Langmuir: the Langmuir isotherm will be simulated for the selected species

OCT Settings

The following settings are specific to the Output Control for Transport (OCT) package:

~	General	
	Ext	.OCT
	Run	Yes
	Translate	Yes
\mathbf{v}	OPTIONS	
	BUDGETCSV	No
~	OPTIONS/PRINT_FORMAT	
	COLUMNS	1
	DIGITS	4
	FORMAT	General
	WIDTH	20

Options

• **BUDGET_CSV** - if this option is set to yes, then a CSV file containing the budget summary similar to what is printed in the list file will be created during the simulation. A budget summary will be printed for each time step in the simulation. This option is set to no by default.

Options/Print Format

The following options relate to the numerical format of the BUDGET_CSV file (if the option is set to yes):

- Columns: the number of columns for writing data
- Digits: the number of digits to use for writing a number
- Width: the number of characters that will be used to write numbers, including white space
- Format: the number format can be: General [default], Fixed, Exponential, or Scientific

10.10.4 MODPATH

The MODPATH program is used for calculating the advective flow pathlines for forward tracking and backward tracking particles. MODPATH has run-time settings for Discharge Options which are used to tell MODPATH what to do with particles when they enter a grid cell where water is leaving the system. Any grid cell where water is leaving the system is classified as a "sink". For example, an extraction well is a sink, or all cells in layer 1 with evapotranspiration are sinks.

Discharge Options

Weak Sink Options

In many cases the water leaving the system through a grid cell is less than the amount of water entering the grid cell. If this difference is small, the cell is classified as a "weak sink". Since MODPATH cannot always determine if a particle should be removed from the system when it encounters a weak sink, there are three options to control how particles should be treated when sinks are encountered.

- Particles always pass through cells with weak sinks
- · Particles are always stopped when they enter cells with internal sinks
- Particles are stopped in the cells where discharge to sinks is greater than a specified total inflow to the cell [default = 5%].

The desired Weak Sink Option may be selected from the Discharge Options window shown in the following figure.

Settings	Translation Log	DIS	LPF	RIV	CHD	RCH	BAS	OC	PCG	NDC	LMT	IN	BT3	DP3	RC3	
<u>⊕</u> Gene	ral		⊿ Dis	charge	•											
🛓 MOD	MODFLOW-2005 Weak Sink Option Particles stop in cells were discharge greater total in									inflow						
🚊 MOD	PATH		Discharge Percentage													
	ischarge Options)		Re	charge O	ptions (IF	RCHTP)		Flux is	assigne	ed to the	e top fa	ce of a	ll cells			
	DMS		Eva	Evapotranspiration Options (IEVTTP)) Flux is assigned to the top face of all cells							
			Weak	Sink O	otion											
				Sink Opti												

Recharge/EVT Options

The Recharge Options are used to define how MODPATH treats the Recharge flow entering the system. The Recharge Options are:

- Recharge flux is treated as internal sources and sinks for all cells
- Recharge flux is assigned to the top face of all cells

The first option treats recharge as a distributed source entering the cell from all sides, while the second option treats recharge as though it is entering only through the top face of the cell.

According to the MODPATH reference manual, the distributed source approximation for areal recharge is usually only appropriate for two-dimensional areal flow models.

The Evapotranspiration Options are the same as described for Recharge above.

10.10.5 MOD-PATH3DU

The mod-PATH3DU program is used for calculating the advective flow pathlines and travel times for forward tracking and backward tracking particles for both finite difference and unstructured grids.

Define Modeling Objectives Define Properties Define Boundary Conditions Select the Next Step Define Observation Wells	Settings Translation Log General	✓ IFACE IFACE(WEL)	0
Define Zone Budget Zones	MODFLOW-NWT	IFACE(CHD)	2
Define Particles	Settings	IFACE(RCH)	6
E Select Run Type	Solvers	IFACE(EVT)	6
Single Run	Recharge and EVT	IFACE(DRN)	6
	Lake Layers	IFACE(RIV)	6
- Run Numerical Engines		IFACE(FHB) IFACE(GHB)	2
	Initial Heads	IFACE(GHB)	6
View Charts	- Anisotropy	IFACE(STR)	6
View Maps	- Output Control	IFACE(MNW2)	0
	H. Advanced Settings	IFACE(MNW)	0
	MOD-PATH3DU	IFACE(CLN)	0
	Settings	V Main	
		OutputPrecision	SINGLE
		ThreadCount	4
		✓ Simulations	
		Mp3duSimulations	(Collection)
		Output Precision Output Precision	

mod-PATH3DU has run-time settings for:

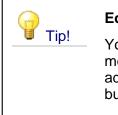
- IFACE: settings to assign boundary condition fluxes to cell faces:
 - o [0] Internal sink/source;
 - [2] Implicit side-face; flow is not explicitly assigned to a cell face, rather mod-PATH3DU distributes the flow to any side faces with zero flow;
 - o [5] Same as MODPATH. Flow through the bottom face of a cell;
 - \circ [6] Same as MODPATH. Flow through the top face of a cell;
 - $\,\circ\,$ [7] Internal sink/source. Flow is assigned to the top face.
- ThreadCount: The number of Threads to use for processing particle tracks

Mp3duSimulations: Opens a dialog for assigning settings for individual particle groups:

Mp3duSimulation Collection Editor			?	\times
Members:	Riv	vers properties:		
0 Rivers	•	₽		
	• ~	General		
		ADAPTIVE_STEP_ERROR	1E-06	
		CAPTURE_RADIUS	1	
		DIRECTION	BACKWARD	
		EULER_DT	0.01	
		GROUP_ID	0000000-0000-0000-0000-00000000	0000
		INITIAL_STEPSIZE	0.1	
		MAX_STEPSIZE	1000000	
		NAME	Rivers	
		SIMULATION_END_TIME	100000000000	
		STAGNATION_DT	0.01	
	~	Options		
		DISPERSION	False	
		RETARDATION	False	
		RUN	True	
		TRACK_TO_TERMINATION	True	
Add Remove				
Aud Nelliove				
			OK Ca	ancel

Each particle group (shown on the left side of the dialog) has the following set of parameters (shown on the right) specified:

- Adaptive Step Error: The error criterion used to determine the maximum allowed error in all directions for the adaptive step size procedure.
- **Capture Radius**: the radial distance from within which a particle will be considered captured by a pumping well.
- **Direction**: this parameter is set when creating/editing the particle group and is disabled.
- Euler DT: the step size below which the Euler method is used instead of the Runge-Kutta method.
- Initial Step Size: The initial particle tracking stepsize
- Max Step Size: The maximum particle tracking stepsize
- Name: The name of the particle group
- **Simulation End Time**: Can be used to overwrite the simulation end time in the model. The default value is the flow model end time for forward simulations and 0 for backward simulation
- Stagnation DT: The tracking size below which a particle is considered stagnated.
- Run: Whether or not Flex will translate and run the particle group
- **Track To Termination**: Track the particles in the group on the last time step until each particle terminates at a boundary or is removed by reaching a stagnation point.



Editing Settings for Multiple Particle Groups

You can select one of more particle groups using the mouse and <SHIFT> or <CONTROL> keys and then adjust these parameters in for the selected groups in bulk.

Please refer to the mod-PATH3DU <u>documentation</u> for more information about the settings listed above.

10.10.6 MT3DMS/RT3D

MT3DMS and RT3D share the same set of available translation settings in Visual MODFLOW Flex since RT3D is effectively a modified version of MT3DMS and shares a common code base. The main differences are that MT3DMS provides more advanced capabilities for simulating dual-domain/sorption modeling while RT3D provides more advanced capabilities for simulating more complex bio-chemical reactions.

The following sections describes the settings for adjusting the solver, advection method, output times, and miscellaneous settings.

- General Settings
- Solution Method
- Output Control
- Advanced Settings

Please Note: SEAWAT is a coupled variable-density flow and transport model that is based on linking modified versions of the MODFLOW-2000 and MT3DMS engines. As such, the translation settings related to transport for MT3DMS also apply to SEAWAT. For more information on the SEAWAT-specific packages see the <u>SEAWAT</u> section.

10.10.6.1 General Settings

Visual MODFLOW Flex supports MT3DMS v.5.1 and RT3D v2.5. The following sections describe the settings for adjusting the solver, advection method, output times, and miscellaneous settings. The translation settings for MT3DMS v5.1 and RT3D v2.5 have the same set of available translation settings in Visual MODFLOW Flex since these two transport engines share a RT3D is effectively a modified version of MT3DMS and shares a common code base. The main difference is that MT3DMS provides more advanced capabilities for simulating dual-domain/sorption modeling while RT3D provides more advanced advanced capabilities for simulating more complex bio-chemical reactions.

Translation Log	DIS	LPF	RIV	CHD	RCH	BAS	OC	PCG	N
eral		⊿ Ge	neral						
FLOW-2005		Por	osity Op	tions			Effecti	ive	
PATH		Cou	urant Nu	mber			0.75		
Discharge Options		Min	. Sat. T	hickness			0.01		
Time Format									
DMS									
Settings									
Solution Method									
Output Control		Porosi	ty Opti	ons					
	eral OFLOW-2005 OPATH	eral PFLOW-2005 PPATH Discharge Options Time Format DMS Solution Method	eral IFLOW-2005 IPATH Discharge Options Time Format DMS Solution Method Discharge Nethod Discharge Nethod Dis	eral IFLOW-2005 IPATH Discharge Options Dime Format DMS Solution Method	eral PFLOW-2005 PATH Discharge Options Dime Format DMS Solution Method	A General PFLOW-2005 IPATH Discharge Options Dime Format DMS Solution Method	A General Porosity Options Discharge Options Dims Dims Dims Bettings Bolution Method	eral IFLOW-2005 IPATH Discharge Options Dime Format DMS Settings Solution Method	eral Image: Constraint of the second secon

Porosity Options

The Porosity options are used to select which porosity measurement to use for the transport solution. For advection-dominated transport, the best choice is to apply the "Effective" porosity option, then diffusion into and out of dead-end pore spaces can be considered negligible. For diffusion dominated transport, the best choice is to select the "Total" porosity option to account for mass transfer to and from dead-end pore spaces.

Courant Number

The Courant number represents the number of cells a particle will be allowed to move through in any direction, in one transport step, when the MOC, MMOC and HMOC methods are used. Generally, the Courant Number is between 0.5 and 1.0; however, values in excess of 1.0 can be used with caution. If the upstream finite-difference method is used, the Courant Number must not exceed 1.0. Since the flow terms in all cells in the entire grid are checked when determining the maximum allowable step size for particle tracking, there may be some cells outside the area of interest with high flow rates. The high flow rates in these cells will control the time step calculation in MT3D. In this situation, setting the Courant Number greater than 1 will not affect the accuracy of the simulation.

Minimum Saturated Thickness as a Fraction of Cell Thickness

The Min. sat. thickness parameter is used to set a value for the minimum thickness of the saturated layer for each cell. This option is particularly important when active cells are running dry. This variable will be in the units specified for length during the initial setup of the model.

10.10.6.2 Solution Method

Select the solution method used to solve the advection-dispersion transport equation.

Settings Translation Log DIS		RIV	CHD	RCH	BAS	OC	PCG	NDC	LMT	IN	BT3	DP3	F		
MODFLOW-2005								Upstream Finite Difference (UFD)							
MODPATH		Use Implicit GCG Solver						le bire	101100 (5.5,					
Discharge Options															
Time Format															
	⊿ G	CG Sett	ings												
Settings	M	ax. numb	er of oute	r iteratior	ns	1									
	M	ax. numb	er of inne	r iteration	IS	50									
• Output Control	Re	Relative convergence criterion					0.0001								
	Co	Concentration change printing interval			0										
		Preconditioners					Jacobi								
			exation Fa			1									
				oss terms			mp all d	ispersio	n cross	terms	to the ri	ght side	e		
			size (DTO			0									
			ze (days)			20	-								
	M	ultiplier				1.1									
	Mar	numbor	of outo	r iterati	000								_		
	MdX.	number	or oute		ULIS										

For numerical solution of the advection-dispersion transport equation, Visual MODFLOW Flex provides the following Solution Methods for the MT3D/RT3D/SEAWAT transport engines:

- Upstream Finite Difference (UFD)
- Central Finite Difference (CFD)
- Higher-order finite-volume TVD method.

No single solution method has been shown to be effective for all transport conditions. The combination of these solution methods, each having its own strengths and limitations, is believed to offer the best approach for solving the most wide-ranging transport problems with desired efficiency and accuracy. A brief description of all the above solution methods, and their advantages and disadvantages, is available below. Further, Zheng and Bennett (1995) provides an introduction to all these solution methods, and a discussion and comparison of their relative strengths and limitations with emphasis on their implications in solving practical problems.

General methodologies of the solution methods

MT3DMS is a transport model for simulating advection, dispersion, and chemical reactions of contaminants in groundwater flow systems. It solves the transport equation after the flow solution has been obtained from groundwater flow model (MODFLOW). The general advective-dispersive equation describing the fate and transport of contaminant of species k in three-dimensional transient groundwater flow systems is:

$$\frac{\delta(\theta C^k)}{\delta t} = \frac{\delta}{\delta x_i} \left[\theta D_{ij} \frac{\delta(\theta C^k)}{\delta x_j} \right] - \frac{\delta}{\delta x_i} \left(\theta v_i C^k \right) \pm \Sigma(q_s C_s^k) \pm \Sigma(R_n)$$

where:

 C^k is the dissolved concentration of species k

 $\boldsymbol{\theta}$ is the porosity of the subsurface medium

t is elapsed simulation time

 x_i is the distance along the respective Cartesian co-ordinate axis

 D_{ij} is the hydrodynamic dispersion coefficient tensor

 v_i

is the seepage or linear pore water velocity. It is related to the specific discharge (q_i) or Darcy flux through the relationship, $v_i = q_i/\theta$

 q_s

is the volumetric flow rate per unit volume of aquifer representing fluid sources (positive) and sinks (negative)

 C_s^k is the concentration of the source or sink flux for species k

 R_n is the chemical reaction term.

All the solution methods listed above treat the dispersion, sink/source, and reaction terms in exactly the same fashion, using the block-centered finite-difference method, either explicit or implicit in time-weighting. They differ; however, in the way the advection term is solved. For instance:

- When one of the particle-based methods (MOC, MMOC, and HMOC) or the Total Variation Diminishing (TVD) method is selected to simulate solute transport, the transport equation is split into two parts. On the left-hand side are the mass accumulation term and the advection term (in fluid mechanics literature, the sum of these two has been referred to as the total derivative of the concentration with respect to time, $\delta C^k / \delta t$). On the right-hand side, the dispersion, reaction, and sink/source terms are represented with finite-difference approximation.
- When the finite-difference methods (UFD, CFD) are used, all terms in the governing equation are treated simultaneously, with all advection, dispersion, reactions, and sink/source terms represented with finite-difference approximations. The finite-difference solution is explicit or implicit-in-time weighting, depending on whether the Generalized Conjugate Gradient Solver (GCG) package is selected or not.

Solution Method

Upstream Finite Difference Method (UFD): Since, the finite-difference method does not involve particle tracking or concentration interpolations, it is normally more computationally efficient than the Method of Characteristics (MOC). In addition, the finite difference method normally has very small mass balance errors because it is based on the principle of mass conservation. However, the Upstream Finite-Difference method can lead to significant numerical dispersion for problems having sharp concentration fronts.

Central Finite Difference Method (CFD): The central finite difference method does not exhibit the numerical dispersion problems like the Upstream Finite Difference method, but is susceptible to excessive artificial oscillations in advection dominated problems.

Third-order Total-Variation-Diminishing Method (TVD): The TVD scheme, which is mass conservative, solves the advection term based on the Universal Limiter for Transient Interpolation Modeling of the Advective Transport Equations (ULTIMATE) algorithm by Leonard (<u>1988</u>). As in the particle-based methods, the TVD scheme solves the advection component independent of the other terms in the transport equation. Results from the TVD scheme may exhibit minor numerical dispersion and minor oscillations in problems having sharp concentration fronts. Since the algorithm is explicit, there is a stability constraint on the step size. The maximum allowed value for the time step is the minimum time step calculated for every active cell.

Please Note: Modifying the default parameter settings for each Solution method requires some understanding of the techniques used to solve the advection-dispersion component of the transport equation. For more details, refer to the MT3DMS User's manual (Zheng and Wang, <u>1999</u>).

Advec tion Metho d	Advanta ges	Disadvantages	Appropriate Conditions
Impli cit Finite Differ ence (<i>with</i> <i>Impli</i> <i>cit</i> <i>GCG</i> <i>solve</i> <i>r</i>)	 Com putati onall y effici ent Mini mal mass balan ce error s Faste r than the expli 	• Numerical dispersion	 Dispersed fronts Peclet number <2

Comparison of Solution Methods

	cit meth od		
Expli cit Finite - Differ ence (<i>with</i> out Impli cit GCG solve r)	 Com putati onall y effici ent Mini mal mass balan ce error s 	 Numerical dispersion 	 Dispersed fronts Peclet number <2
Total Varia tion Dimi nishi ng (TVD)	 Mass cons ervati ve Most accur ate 	 Numerical dispersion (minimal) Longer runtimes 	

Using the GCG Solver

When the GCG Solver Package is specified to be included in a simulation, MT3D will do the following:

- When the finite-difference methods (UFD, CFD) are used, all terms in the governing equation are represented with implicit-in-time weighted finite-difference approximations.
- When the TVD method (or the particle-based methods MOC, MMOC and HMOC) are used to simulate solute transport, the terms on the right-hand side are represented with implicit-in-time weighted finite-difference approximations. The TVD algorithm implemented in MT3D is explicit-in-time. This means that even if the GCG Package is used, the time steps in the TVD run will still be subject to a time constraint - but only the advection term.

If the GCG solver is not included, then all terms are represented with explicit-in-time weighted finite-difference approximations.

When the GCG Solver is included, during translation the GCG package file (projectname.GCG) will be created in the model run directory.

GCG Solver Settings

Maximum number of outer iterations (MXITER) [Default = 1]: The outer loop in the iteration process updates all the coefficients that are concentration-dependent. The default number of outer iterations is one. It should be set to an integer greater than one only when a non-linear sorption isotherm is included in simulation. For further detail please refer to page 4-19 in the MT3DMS Documentation and User's Guide.

Maximum number of inner iterations (ITER1) [Default = 50]: The inner loop in the iteration process continues to iterate toward the solution until the convergence criterion is obtained or the maximum number of inner iterations is reached. During these iterations, the coefficient matrix and the right hand side vector matrix remain unchanged. The default number of inner iterations is fifty. A maximum value of thirty to fifty inner iterations should be sufficient for most problems. For further details please refer to page 4-19 in the MT3DMS Documentation and User's Guide.

The Relative convergence criterion (CCLOSE) [Default = 10^{-4}]: is used to judge the convergence, in terms of relative concentration, of the inner iterations of the solver. The default value is 10^{-4} . A value between 10^{-4} and 10^{-6} is generally adequate.

The Concentration change printing interval (IPRGCG) [Default = 0]: is the interval for printing the maximum concentration changes of each iteration. The default is 0 for printing at the end of each stress period.

Preconditioners

The GCG Solver implicitly solves the non-advective terms in the transport equation using a two-iteration loop process and the choice between three pre-conditioning options:

- Jacobi (ISOLVE=1)
- SSOR (ISOLVE=2)
- Modified Incomplete Cholesky (ISOLVE=3)

The Modified Incomplete Cholesky method usually converges faster than the other two method options, but it requires significantly more memory. If SSOR is chosen, you must specify a relaxation factor.

Dispersion tensor cross terms

The GCG Solver has two options for dealing the cross-derivative terms of the dispersion tensor:

• Lump all dispersion cross terms to the right hand side (NCRS=0) will place all the dispersion tensor cross terms to the right hand side of the matrix equation and consider them as known values. This method approximates the equation (the loss of accuracy is generally insignificant) but is highly efficient (reduces the memory requirement by nearly two thirds) since there are significantly less unknown terms to be solved. For further detail please refer to the MT3DMS Documentation and User's Guide.

 Include full dispersion tensor (NCRS=1) will keep all the dispersion tensor cross terms on the left-hand side of the matrix equation and consider them as unknown terms. This method gives the exact matrix equation but is memory intensive since there are significantly more unknown terms to be solved. For details, refer to the MT3DMS Documentation and User's Guide.

Initial Step Size (DT0):

[Default = 0]: The Initial Step Size is used to override the automatically calculated initial time step. The user can assign a value to be used for the first iteration of the solution. The default value of 0 means that the MT3D calculated value will be used.

Please Note: If the implicit solver is not selected, then this value will be ignored and the value for DT0 will be taken from the Output Control settings.

Maximum transport step size (TTSMAX)

[Default = 0]: This value is the maximum time step size allowed when a multiplier greater than 1 is used. Setting this equal to zero imposes no maximum limit.

Multiplier (TTSMULT)

[Default = 1]: This is the multiplier used to calculate the size of the next transport time step when the finite difference method is used with the implicit GCG solver. A value between 1 and 2 is generally adequate. Using a time step multiplier will degrade the solution at later times when the timestep becomes large, but can significantly decrease the amount of time needed for the solution. If one of the particle-based methods or the TVD method is used, this value will be ignored.

10.10.6.2.1 Technical Review

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Overview of MT3D Solution Methods

MT3D offers two general options for simulating solute transport:

- 1. When the "pure" finite difference methods are used (FD), all terms in the governing equation are treated simultaneously, with advection, dispersion, reactions, and source-sink mixing terms represented with finite-difference approximations.
- 2. When the operator-splitting methods are used to simulate solute transport, the governing equation is split into two parts. On the left-hand side are the mass accumulation term and the advection term (in the fluid mechanics literature, the sum of these two is referred to as the total derivative of the concentration with respect to time, Dc/Dt). On the right-hand side, the dispersion, reactions, and source-sink mixing terms are represented with finite-difference approximations. The operator-splitting techniques implemented in MT3D are the particle-based methods (MOC, MMOC and HMOC) and a 3rd-order TVD method.

Treatment of the transport terms with respect to time

MT3D offers the user two options for evaluating the terms in the finite-difference approximations, explicit or implicit-in-time weighting:

- **1. Explicit-in-time weighting.** With explicit-in-time, or forward-in-time weighting (FIT), the terms in the finite-difference approximations are evaluated at the previous time step. This was the only option available in versions of MT3D from v.1.1 to MT3D96. Explicit-in-time weighting has the advantage of not requiring the assembly, storage, and solution of a matrix. It requires the least amount of RAM of all feasible methods. In particular, it requires no additional RAM with respect to the corresponding MODFLOW model. This was an important requirement for the development of MT3D, since the code was developed on a PC, for implementation on PCs. We now live in a world in which RAM is inexpensive. However, when MT3D was developed in 1987-1988, additional RAM over 640 KB was very limited and very expensive. Explicit-in-time weighting has the disadvantage of not being stable unless tight restrictions on the size of time steps are satisfied. In many cases, the size of the time steps can be relatively small - and may only get smaller as the spatial resolution of a model was increased. Furthermore, in versions of MT3D preceding MT3D96, the calculation of the overall maximum allowable step size was not correct, and a model could still experience severe problems although it seemed that all stability criteria were being satisfied. In theory, the maximum Courant number may be 1.0. However, because the stability requirements were not calculated correctly, in practice users often had to specify maximum Courant numbers significantly smaller than 1.0 to ensure stability.
- 2. Implicit-in-time weighting. With implicit-in-time, or backward-in-time weighting (BIT), the terms in the finite-difference approximations are evaluated at the current time step. This option was added with the introduction of MT3DMS and MT3D99. Implicit-in-time weighting has the advantage of being unconditional stable, and allows the use of relatively large time steps. The option requires the assembly, storage, and solution of a matrix, but these requirements are not as onerous as they were, both because additional RAM is relatively inexpensive, and because accurate and efficient matrix solvers are now widely available. The disadvantage of the method is that it is now possible to create transport models that require much more storage than the corresponding MODFLOW model. Although implicit-in-time weighting is unconditionally stable, its accuracy is not assured if the time steps are too large. In order to guarantee the accuracy, the maximum Courant number may be limited to 1.0. As a simulation proceeds and the concentration gradients diminish, this requirement may be relaxed.

Time-weighting options with the particular MT3D solution methods

- 1. When the "pure" finite difference methods are used (FD), all terms in the governing equation may be represented with either explicit or implicit-in-time weighted finite-difference approximations.
- 2. When the particle-based methods (MOC, MMOC and HMOC) and the TVD method are used to simulate solute transport, the terms on the right-hand side (the dispersion, reactions, and source-sink mixing) may be represented with either explicit or implicit-in-time weighted finite-difference approximations.

A potential source of confusion to MT3D users is the apparent absence of a switch for specifying explicit or implicit time weighting. It turns out that this switch is 'implied'. When the user specifies that the GCG Solver Package is to be included in a simulation, the user is telling MT3D to do the following:

- 1. When the "pure" finite difference methods are used (FD), all terms in the governing equation are represented with implicit-in-time weighted finite-difference approximations.
- 2. When the particle-based methods (MOC, MMOC and HMOC) and the TVD method are used to simulate solute transport, the terms on the right-hand side are represented with implicit-in-time weighted finite-difference approximations. At the risk of confusing the issue, I should add at this point that the TVD algorithm implemented in MT3D is explicit-in-time. This means that even if the GCG Package is used, the times steps in TVD run will be still be subject to a time constraint but only the advection term.

If the user does not specify the use of the GCG package, then all terms are represented with explicit-in-time weighted finite-difference.

10.10.6.3 Output Control

The Output Settings and Output Times settings are used to define the length of the transport simulation and the times at which the results will be saved to the binary concentration file (.UCN).

Settings	Translation Log	DIS	LPF	RIV	CHD	RCH	BAS	OC	PCG	NDC	LMT	IN		
🕀 Gen	⊞. General				⊿ General									
MOE 🗄	. MODFLOW-2005				Simulation time length (project time units)									
MOE 🖷	- MODPATH				Max number of transport steps									
	Discharge Options				Specify maximum step size									
· · · ·	Time Format				Maximum step size (project time units)									
📗 📥 МТЗ	DMS	Sa	Save concentation at observation point for every Nth time step											
	Settings	Save one-line summary of mass budget for every Nth time step												
	Solution Method			Save CMB/CCM file (mass balance output)										
. (Output Control													
	- Output Setting													
	Output Times													
			Simul	ation tin	ne lengt	h (proje	ct time	units)						

Simulation time is the total length of the transport simulation in the specified time units. This must be greater than zero.

Max # of transport steps is the maximum number of transport steps for the simulation. Once the simulation has run through the specified Max # of transport steps the model will stop. This parameter is primarily used to limit the size of the output files generated.

Specify max stepsize sets the maximum step size to use for each transport time step. MT3D will use the smaller of: the internally calculated maximum timestep size based on the Courant number, or the maximum timestep size specified here. If the implicit GCG solver is used, this value is ignored and the value found in the GCG Solver options is used instead.

Save concentration at observation point for every Nth time step allows to filter the amount of observation data that is saved to the .OBS file; ideal for transient runs with large output files

Save one-line summary of mass budget for every Nth time step allows to filter the amount of mass budget data that is saved to the .MAS file; ideal for transient runs with large output files

The Save .CBM/.CCM file option must be checked if you want Mass Balance output to be saved (for example, to generate Zone Budget-Transport data).

Output Times

In the grid shown below, you can enter the output times for which you want MT3DMS to save during the run. The simulation results are saved in the MT3D output *.OT file.

The toolbar above this grid provides the following options (from left to right)

- Add row to the grid
- Delete selected row(s)
- · Copy selected rows to clipboard
- Paste from clipboard: ideal if you have times defined in a column in an Excel spreadsheet, or in a text file (one time entry per row)

Settings	Translation Log	DI	S	LPF	RIV	CHD	RCH	BAS	OC	PCG	NDC	LMT
General MODFLOW-2005			-	×	G ñ							
										Time		
Discharge Options Discharge Options Time Format MT3DMS Settings Solution Method Output Control Output Settings Output Times				1								
				7	730							
				1	460							
				2	2190							
				2	2920							
		s		3	8650							
					5475							
					7300							
				1	300							

10.10.7 SEAWAT

Visual MODFLOW Flex supports SEAWAT v.4.00.05 - which based on a tight coupling of MODFLOW-2000 and MT3DMS. As such, the translation settings are very similar to the settings for MODFLOW and MT3DMS and largely follow the same format:

- settings and packages related to flow can be found under the SEAWAT node (refer to MODFLOW settings for details).
- settings and packages related to solute transport can be found under the SEAWAT Transport node (refer to the <u>MT3DMS/RT3D</u> settings).

 the SEAWAT-specific variable density flow (<u>VDF</u>) and viscosity (<u>VSC</u>) package settings can also be found under the SEAWAT Transport node

Please Note: the VSC package is only compatible with LPF as the selected internal flow package.

🖃 General
<mark>Settings</mark> ⊡- SEAWAT
E- SEAWAI
Settings
Solvers
···· Recharge and EVT
Lake
Layers
···· Rewetting
···· Initial Heads
Anisotropy
Output Control
Settings Solvers Solvers Careeral Solvers Solvers Careeral Solvers So
SEAWAT Transport
General
Solution Method
Output Control
Advanced Settings
ADV
BTN
DSP
GCG
LMT
BCT
SSM
···· VDF
VSC

SEAWAT Flow Engine Settings

- <u>General</u>
- <u>Settings</u>
- <u>Solvers</u>
- <u>Recharge and Evapotranspiration</u>
- Lakes
- Layer Types
- <u>Cell Rewetting</u>
- Initial Heads
- <u>Anisotropy</u>
- Output Control
- Advanced Settings

SEAWAT Transport Engine Settings

General Settings

- Solution Method
- Output Control
- VDF Package
- VSC Package

10.10.7.1 DSP Package

The Dispersion (DSP) package is an integral package of all transport engines as it defines the dispersivity and diffusivity terms used in the governing transport equation. For most groundwater solutes, the molecular diffusion term is relatively small compared to the magnitude of the dispersivity terms and a single value for multi-species is generally acceptable. However, SEAWAT may be used to simulate (salt) solute and heat transport simultaneously. In such cases, the diffusion term for the heat "solute" is used to represent thermal conductance (Langevin, et al, 2007) which occurs at higher magnitudes such that species-dependent "diffusion" parameters may be desired. As such, the advanced translation settings for the DSP package includes a setting to enable multi-species diffusion:

🖃 - General	✓ General		
Settings	CUnit	60	
EAWAT SEAWAT	Ext	.DP3	
SEAWAT Transport	LUnit	70	
General	Run	Yes	
Solution Method	Translate	Yes	
Output Control	✓ DSP		
Advanced Settings	Multi-Diffusion	True	
GCG LMT RCT SSM VDF VSC			
	Multi-Diffusion		

10.10.7.2 VDF Package

The Variable Density Flow (VDF) package is an integral part of the SEAWAT engine as it defines the relationship(s) between fluid density and solute concentration(s). The VDF package is required to run a SEAWAT model simulation. Numerous options and settings are supported as part of the translation settings in Visual MODFLOW Flex and are described below.

Settings for the VDF package are divided into <u>high-level settings</u> that are always required as part of the VDF package and <u>low-level settings</u> that are required (or not) based on the high-level settings. High-level settings are located in the VDF group of the advanced package table, while low-level settings are displayed as needed in the form area below. For more complete explanation of the input settings for the VDF package, please refer to p16-19 of the SEAWAT V4 Manual (Langevin *et. al.*, 2007).

Settings Translation Log		
- General	✓ General	
Settings	CUnit	57
E- SEAWAT	Ext	.VDF
Settings	LUnit	67
Solvers	Run	Yes
Recharge and EVT	Translate	Yes
Lake	V VDF	
Layers	Density option	Calculate density from multiple species
Rewetting	Internodal density calculation algorithm	Central-in-space algorithm
Initial Heads	Variable density water table correction	Applied
Anisotropy	Initial time step	0.01
Output Control		
Advanced Settings		
SEAWAT Transport	Implicit coupling using DNSCRIT	
General	Explicit coupling with one iteration	
Solution Method		
Output Control	Explicit coupling with multiple iterations	
Advanced Settings	Maximum number of implicitly coupling iterations for VDF and	IMT
ADV	20	
BTN		
DSP	Minimum Fluid Density Maximum Fl	uid Density
GCG		
LMT	0 🚖 kg/m^3 0	★ kg/m ³
RCT	Reference Fluid Density	
SSM	1000 ¢ kg/m^3	
VDF	TUUU Rynn 3	
VSC		
	Fluid density convergence criterion	
	0.0001 kg/m^3	
	Density vs pressure head slope	
	0.00446 🚖 kg/m^3/m	
	Reference pressure head	
	0 🔶 m	

Variable Density - Theory

In SEAWAT, fluid density is estimated as a linear function of the concentration of one or more solute species, temperature, and pressure head:

$$\rho = \rho_{(ref)} + S \delta \rho / \delta C_{i} \cdot [C_{i} - C_{i (ref)}] + \delta \rho / \delta T \cdot [T - T_{(ref)}] + \delta \rho / \delta \ell \cdot [\ell - \ell_{(ref)}]$$

where:

 $\underline{\rho}$ is the fluid density [M/L³]

 $ho_{\text{(ref)}}$ is the reference fluid density [M/L³]

 C_i is the concentration of the ith species [M/L³]

 $C_{i (ref)}$ is the reference concentration, or the concentration at which the fluid density = $\rho_{(ref)}$ [M/L³]

 $\delta \rho / \delta C_i$ is the density/concentration slope, or change in density per unit change in solute concentration of the ith species [-]

T is the temperature [T]

 $T_{(\text{ref})}$ is the reference temperature, or the temperature at which the fluid density = $\rho_{(\text{ref})}$ [T]

 $\delta \rho / \delta T$ is the density/temperature slope [M/L³·T]

ℓ is the pressure head [L]

 $\boldsymbol{\ell}_{(\text{ref})}$ is the reference pressure head, or the pressure head at which the fluid density = $\rho_{(\text{ref})}$ [L]

 $\delta \rho / \delta \ell$ is the density/pressure head slope [M/L⁴]

Variable	Reference Value	Slope	Setting Location			
Density	1,000 kg/m ^{3*}	n/a	VDF Translation Settings			
Salt Concentrat ion	0 mg/L	0.714				
Temperatu re	25 ⁰C	-0.375 kg/m³ / °C				
Pressure Head	0 m	4.46x10 ⁻³ kg/m ⁴	VDF Translation Settings			
Source: Lar	Source: Langevin et al. (2007)					

Commonly used values for the VDF package

*See Table A.2 in Viessman and Lewis (2003) or similar hydrology/engineering reference textbook for more precise values

VDF High-Level Settings

Density Option

The density option is a flag (MT3DRHOFLG) that defines which species contribute to the relationship of concentration-derived variable fluid density. The options are:

- Calculate density from salt only: salt is assumed to be the first species as defined in the modeling objectives [MT3DRHOFLG=1] [default]
- Calculate density from multiple species: species defined with non-zero density slope values as defined in the modeling objectives will be included in the variable density calculations [MT3DRHOFLG=-1]
- Uncoupled simulation using pre-calculated density: density will be estimated using input values from a specified .UCN file [MT3DRHOFLG=0]

Internodal Density Calculation Algorithm

The Internodal Density Calculation Algorithm is a flag (MFNADVFD) that determines the method for calculating the internodal density values used to conserve fluid mass. The options are:

- central-in-space algorithm (MFNADVFD = 2)
- upstream-weighted algorithm (MFNADVFD = 0)

Variable Density Water Table Correction

This option represents a flag (IWTABLE) that is used to activate the variable-density watertable corrections (Guo and Langevin, <u>2002</u>).

- correction applied (IWTABLE = 0)
- correction not applied (IWTABLE = 1)

Initial Time Step

A variable for the length of the first transport timestep, used to start the simulation if both of the following two conditions are met: 1) the IMT Process is active, and 2) transport timesteps are calculated as a function of the user-specified Courant number (the MT3DMS input variable, PERCEL, is greater than zero)

VDF Low-Level Settings

Coupling Iteration Radio Selection (NSWTCPL)

If the model simulation is setup to dynamically calculate variable density flow (i.e. MT3DRHOFLG<>0), then this option sets the parameters that define the feedback link that between flow and transport caused by the relationship between solute concentrations and fluid density. The options are as follows:

- Implicit coupling using DNSCRIT density is only (re)calculated:
 - o at the first transport step of the simulation,
 - o at the last transport step of a given MODFLOW timestep, or
 - when the maximum density change at a cell is greater than the <u>fluid density</u> <u>convergence criteria</u>
- Explicit Coupling with one iteration flow and transport will be explicitly coupled using a one-timestep lag.
- Explicit Coupling with multiple iterations flow and transport will be explicitly coupled using a one-timestep lag. Density will be recalculated up to is the maximum number of non-linear coupling iterations for the flow and transport solutions.

Please Note: The explicit coupling option is normally much faster than the iterative option and is recommended for most applications

Maximum Number of implicitly coupling iterations (NWSTCPL)

SEAWAT will stop execution if the maximum number of iterations has been reached and convergence between flow and transport has not occurred.

Minimum/Maximum Fluid Density

Calculated density values will be truncated if they fall below the minimum fluid density or above the maximum fluid density. If a value of zero is entered for the minimum and maximum fluid density, then SEAWAT will *not* truncate to a lower and an upper range of calculated density values, respectively.

Reference Fluid Density

The reference fluid density is the density at the reference concentration, temperature, and pressure. See <u>Theory</u> Section above.

Fluid Density Convergence Criteria (DNSCRIT)

The fluid density convergence criteria (DNSCRIT) is a user-specified density value [M/L³]. If explicit coupling with multiple iterations is selected, then DNSCRIT is the convergence criterion, in units of fluid density [M/L³], for convergence between flow and transport. If the maximum fluid density difference between two consecutive implicit coupling iterations is not less than DNSCRIT, the program will continue to iterate on the flow and transport equations, or will terminate if NSWTCPL is reached. If implicit coupling is selected, DNSCRIT is the maximum density threshold, in units of fluid density. If the fluid density change (between the present transport timestep and the last flow solution) at one or more cells is greater than DNSCRIT, then SEAWAT will update the flow field (by solving the flow equation with the updated density field).

Density vs Pressure Head Slope (DRHODPRHD)

Density vs Pressure Head Slope (DRHODPRHD) is the slope of the linear equation of state that relates fluid density to the height of the pressure head (in terms of the reference density). A value of zero, which is typically used for most problems, inactivates the dependence of fluid density on pressure. See <u>Theory</u> Section above.

Reference pressure head (PRHDREF)

Reference pressure head (PRHDREF) is the reference pressure head. This value should normally be set to zero. See <u>Theory</u> Section above.

Uncoupled Simulation Pre-calculated Density Options

If the <u>Density Option</u> is set is set to uncoupled (MT3DRHOFLG=0), then you will have the option of using:

- the reference fluid density or
- density from a .UCN file

If choosing the latter option, you can enter or browse to .UCN file that contains the densities to be used. The .UCN file must be based on a grid of the same dimensions and have the same number of timesteps as the simulation in which it is to be used.

_	Use reference density	
0	Use density from UCN file	
		Browse

10.10.7.3 VSC Package

The Viscosity (VSC) package is the package in <u>SEAWAT</u> that defines the relationship between solute concentration(s) and temperature with viscosity. The VSC package is optional to run a SEAWAT model simulation and can be turned off by setting Run=No in the advanced settings, if desired. Numerous options and settings are supported as part of the translation settings in Visual MODFLOW Flex and are described below.

For a more complete explanation of the input settings for the VSC package, please refer to p20-22 of the <u>SEAWAT V4 Manual</u> (Langevin, *et. al.*, <u>2007</u>). The theoretical basis of how viscosity is used in SEAWAT is discussed on page 6 of the SEAWAT V4 Manual.

Please Note: The VSC package can only be used with the LPF internal flow package.

Settings Translation Log					
🖃 General	✓ Gener	al			
Settings	CUnit		65		
SEAWAT	Ext		.VSC		
Settings	LUnit		75		
Solvers	Run		Yes		
···· Recharge and EVT	Transla	te	Yes		
Lake	✓ VSC				
Layers	Viscosit	y option	Calculate viscosity from	n temperature and multiple sp	pecies
Rewetting					
Initial Heads					
Anisotropy					
Output Control	Minimum V		Maximum Visc	· · · · · · · · · · · · · · · · · · ·	^
Advanced Settings	0	🚖 kg/m/da	у 0	🚖 kg/m/day	
SEAWAT Transport	D-(10			
General	Reference	· ·			
Solution Method	0.000894	🚖 kg/m/da	у		
Output Control					
Advanced Settings		linear relation			
ADV	Voss (984) parametrization			
BTN DSP		vski (1991) parametrization	_		
GCG					
LMT	Guo ar	nd Zhao (2005) parametriz	ation (not applicable for wate	r)	
BCT		Name	Value	Unit	1
SSM			2.394E-05		
VDF	•	A1_18		kg/m/d	
VSC		A2_18	10		
		A3_18	248.37		
		A4_18	133.15		
					~

Viscosity - Theory

Unlike fluid density, a linear approximation of viscosity does not adequately represent the effect of temperature over the range of typical/natural conditions on dynamic viscosity. For this reason, an alternative equation for dynamic viscosity has been implemented in SEAWAT:

$$\boldsymbol{\mu} = \boldsymbol{\mu}_{(\text{ref})} + \boldsymbol{S} \boldsymbol{\delta} \boldsymbol{\mu} / \boldsymbol{\delta} \boldsymbol{C}_{i} \cdot [\boldsymbol{C}_{i} - \boldsymbol{C}_{i \, (\text{ref})}] + \boldsymbol{\mu}(\boldsymbol{T})$$

where:

 μ is the fluid dynamic viscosity⁻ [M/L·T]

 $\mu_{\mbox{\tiny (ref)}}$ is the reference fluid dynamic viscosity [M/L·T]

 C_i is the concentration of the ith species [M/L³]

 $C_{i (ref)}$ is the reference concentration, or the concentration at which the fluid viscosity = $\mu_{(ref)}$ [M/L³]

 $\delta\mu/\delta C_i$ is the viscosity/concentration slope, or change in viscosity per unit change in solute concentration of the ith species [L²/T]

T is the temperature [T]

 $\mu(T)$ is the viscosity/temperature function - see below.

* **Note**: The governing equations implemented in SEAWAT use dynamic viscosity. For simplicity, subsequent references to viscosity refer to dynamic viscosity (rather than kinematic viscosity).

Values for the viscosity/concentration slope for each species ($\delta\mu/\delta C_i$) and the reference concentrations ($C_{i \text{ (ref)}}$) are set at the Define Modeling Objectives Step (if variable density is the selected flow type). The available/published empirical relationships between viscosity and temperature are tabulated below:

Option	Equation	A ₁	A ₂	A ₃	A4	A5
Linear	$\mu(T) = \frac{\partial \mu}{\partial T} \cdot \left(T - T_{(ref)}\right)$					
Voss (1984)	$\mu(T) = A_1 \cdot A_2^{\left(\frac{A_3}{T+A_4}\right)}$	2.934 x 10 ⁻⁵	10	248.37	133.15	
Pawlowski (1991)	$\mu(T) = A_1 \cdot [A_2 + A_3 \cdot (T + A_4)]^{A_5}$	1.0 x 10 ⁻³	1	l.5512 x 10 ⁻²	-20	-1.572
Guo and Zhao (2005)*	$\mu(T) = A_1 \cdot T^{A_2}$	0.168				

Temperature/Viscosity Functions available in the VSC package

Source: after Langevin et al. (2007)

NOTES:

- all equations are based on base units of L=meters, M=kilograms, T =degrees Celsius
- Guo and Zhao (2005) is applicable to oil rather than water at a temperature range of 5°C ≤ T ≤ 170°C.

Viscosity - Settings

Viscosity Option (MT3DMUFLG)

The viscosity option is a flag (MT3DMUFLG) that defines which species contribute to the relationship of concentration-derived variable fluid viscosity. The options are:

- Calculate viscosity from salt only: salt is assumed to be the first species as defined in the modeling objectives [MT3DMUFLG=1] [default]
- Calculate viscosity from multiple species: species defined with non-zero viscosity slope values as defined in the modeling objectives will be included in the viscosity calculations. This option also enables more advanced options to model the effects of temperature on viscosity [MT3DMUFLG=-1]
- Use specified viscosity: viscosity will be estimated using a default value or input values from a specified .UCN file [MT3DMUFLG=0]

Minimum/Maximum Fluid Viscosity (VISCMIN/VISCMAX)

Calculated viscosity values will be truncated if they fall below the minimum fluid viscosity or above the maximum fluid viscosity. If a value of zero is entered for the minimum or maximum fluid viscosity, then SEAWAT will *not* truncate to a lower or upper range of calculated viscosity values, respectively.

Reference Viscosity (VSCREF)

The reference fluid viscosity is the viscosity at the reference concentration and temperature.

Viscosity vs. Temperature

If a species has been designated as the temperature species as part of a variable density simulation at the Define Modeling Objectives and the Viscosity Option is set to calculate viscosity from multiple species, then the viscosity vs. temperature options described in the <u>theory</u> section above will be shown:

Pawlo	owski (1991) parametri:	zation	
Guo a	and Zhao (2005) paran	netrization (not applicable for w	ater)
	Name	Value	Unit
•	A1_18	2.394E-05	kg/m/d
	A2_18	10	
	A3_18	248.37	
	A4_18	133.15	

In this case, you may select one of the four viscosity/temperature relationships: Simple linear, Voss (1984), Pawlowski (1991), or Guo and Zhang (2005). The table below will be

populated with the associated number of fitting parameters ($A_1 - A_5$, as applicable) set to the respective defaults.

Specified Viscosity Settings

If the <u>Viscosity Option</u> is set is set to uncoupled (MT3DMUFLG=0), then you will have the option of using:

- the reference viscosity,
- read specified viscosity from a .UCN file
- read concentration from .UCN file and convert to viscosity using linear expression

If choosing either of the last two options, you can enter or browse to .UCN file that contains the file to be used for the respective option. The .UCN file must be based on a grid of the same dimensions and have the same number of timesteps as the simulation in which it is to be used.

۲	Values for viscosity will be set to VISCREF for 1st stress period. The next stress period will reuse viscosity from the previous period.	
0	Read specified viscosity from UCN file	
		Browse
0	Read concentration from UCN file and convert to viscosity using linear expression	
		Browse

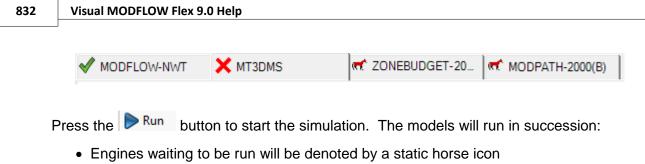
10.11 Run Numerical Engines

At this step, you can run the set of engines selected at the Single Run step.

The Run button will run the selected numeric engines using the required data files already present in the project folder the were generated at the <u>Translation</u> Step. If the required files are not present in the project folder, the numeric engines will not run. A warning message will appear indicating that the Visual MODFLOW files will not be translated prior to running the model.

Starting a Model Run

At the Run Numerical Engines Step, separate tabs will be generated for each engine or postprocessing utility selected at the single run step. The particle tracking utilities may generate multiple tabs depending on the number and type of particle groups to be simulated:

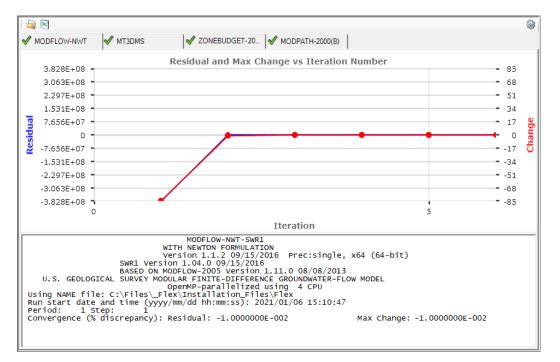


- The currently active engine or utility will be denoted by a running horse icon
- Engines that have successfully completed will be denoted by a green checkmark
- Engines that failed to run or ran with errors will be denoted by a red "x"

Model Run Progress

During a flow and/or transport engine run, Visual MODFLOW Flex will provide feedback on the progression of the model run in a text console. By default, Visual MODFLOW Flex will also display an optional chart with the solution progress by iteration reported by the engine's solver, including:

- the global residual error and/or
- the maximum change in the heads or concentrations relative to the previous iteration



Note that MODFLOW-6 models will show one chart for each model included in the solution (e.g. a groundwater flow model (GWF) solution and one groundwater transport model (GWT) solution for each species)

Chart Controls

The chart can be toggled on and off by clicking the plot button (\boxtimes). You can also change the display settings the chart by clicking the Run View Settings button (\circledast):

🔡 Run View Settings	×
Iterations to Display ○ All ④ Specified 300 ←	
Dynamic Rescaling	
Reduce scale after 50 + iterations have values that are less than half the current scale.	
OK Cancel	

Iterations to Display - allows you to select how many iterations to show. If a specified number is selected, then only that many of the most recent iterations will be displayed

Dynamic Rescaling - allows you to select whether the vertical axes of the chart will be rescaled after a given number of iterations

Model Run Completion

When the run completes additional information including the run time and other diagnostics will be to the text console of each engine. Model output will also be added to Run > Output folder in the Model Explorer:

Flow Engine Outputs

The following nodes will be added to the Output folder on the Model Explorer:

- Heads,
- Drawdown,
- Flooded Cells,
- Budget,
- Velocity, and
- Water Table

A saturation node will also be added if an unsaturated flow model is run (using MODFLOW-SURFACT or the UZF package). One or more residuals nodes may be added if head or flow observations were added to the run.

Transport Engine Outputs

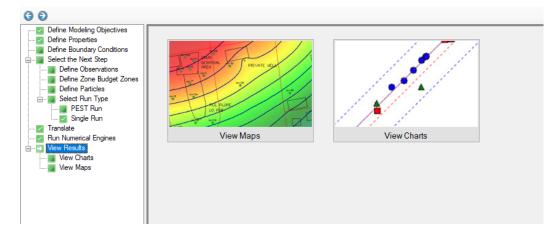
One node will be added per simulated species for simulations including groundwater transport (e.g. using MT3D-MS, RT3D, SEAWAT, or MODFLOW-SURFACT with transport). A separate node for each species will also be added for the immobile domain if sorption is included in the Modeling Objectives. One or more residuals nodes may be added if concentration observations were added to the run.

Particle Tracking Outputs

One node will be added per particle group with pathline information if particle tracking was included as part of the simulation.

When you have finished reviewing the model run results, click 💟 (Next Step) button to proceed to the View Results step.

10.12 View Results



At the View Results step, you have the option to <u>View Maps</u> or <u>View Charts</u>.

View Maps

At the <u>View Maps</u> step, you can visualize many different types of model outputs:

- Heads, drawdown, budget, velocity water table, flooded cells;
- Residuals (if observations were included in the simulation);

- Pathlines (if particle tracking was included in the simulation); and
- Concentrations (if transport was included in the simulation).

View Charts

At the <u>View Charts</u> step, you can visualize results in a variety of chart types:

- Calibration Dashboard
 - o Observed vs. Calculated Heads
 - o Time Series
- Mass Balance
- Zone Budget

10.12.1 View Maps

Following a successful model simulation, outputs are generated and Outputs branch in the Model Explorer tree for the active run.

- Flow Engine Outputs
 - o Heads and Drawdown
 - o Budget
 - o <u>Velocity</u>
 - o Water Table
 - o Flooded Cells
 - o <u>Residuals</u>

Pathlines

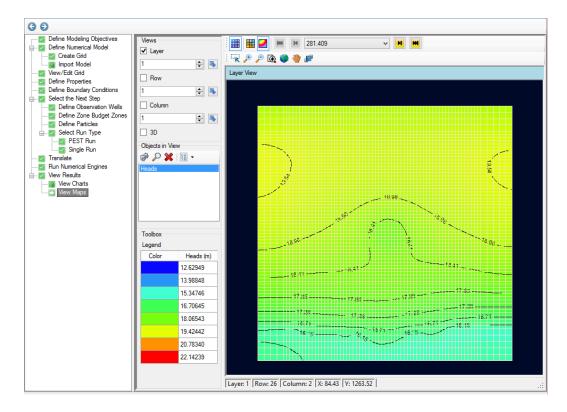
- Transport Engine Outputs
 - o Concentrations
 - o Concentration Residuals

Flow Engine Outputs

Upon successful completion of a flow engine simulation, heads and related outputs can be visualized at the View Maps step as discussed below.

Heads and Drawdown

At the View Maps step, you can view contours and color shading of the flow engine results.



By default, you will see color shading and contours of the calculated heads, in layer view. You can display heads along a row, and along a column, and in 3D, using the same tools as you used earlier.

If your model is transient, use the time controls above the Flex Viewer to change the output time; as you do this, all active viewers (layer, row, column, 3D), will refresh to show the heads for the new output time.

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The display settings (color classes, contour line intervals, etc.) for the Layer, Cross-section, or 3D views can be adjusted in the Style settings. To load these settings, right click on Heads or Drawdown in the Outputs section of the Model Explorer, and select "Settings". For more details about these settings, see the section on <u>3D Gridded Data Settings</u>.

Budget

At the View Maps step, you can view cell-by-cell flows (read from the MODFLOW .BGT file). Once displayed in the viewer, load the Style settings for Budget, and choose the desired display type (Cells is turned on by default). Under the Colors panel (shown below), you can select from various Budget attributes:

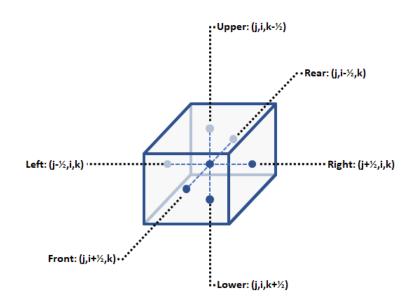
- XRate: lateral flow into the cell from the right and left face (adjacent columns)
- YRate: lateral flow into the cell from the front and rear face (adjacent rows)
- ZRate: vertical flow into the cell from cells in the upper and lower layer face (adjacent layers)

- InFlowRate: total flow into the cell from all adjacent cells
- OutFlowRate: total flow out of the cell from all adjacent cells
- NetFlowRate: InFlowRate OutFlowRate
- One term will be also added for each active boundary condition type with external flows in the model simulation (e.g. Wells, Drains, Recharge, Constant Heads, Rivers, etc.).

Calculation Cell Flow-in/ Flow-out Based on Inter-Cell Flow Terms

Inter–cell flow terms are saved in the output budget file (.BGT) for three neighbors of a given cell(j,i,k):

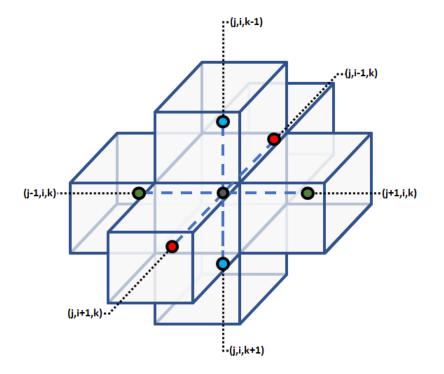
- RIGHT FACE (j+½,i,k)
- FRONT FACE (j,i+½,k)
- LOWER FACE (j,i,k+½)



Indices for the six adjacent cell faces surrounding cell j,i,k.

The inter-cell flows for the remaining three faces are given by:

- LEFT FACE(j-½,i,k) = RIGHT FACE([j-1]+½,i,k)
- FRONT FACE(j, $i+\frac{1}{2}$,k) = REAR FACE(j, $[i-1]+\frac{1}{2}$,k)
- UPPER FACE(j,i,k+½) = LOWER FACE(j,i,[k-1]+½)



Indices for the six adjacent cells surrounding cell j,i,k. Adapted from MODFLOW-2005 Users Manual, USGS Publication TM6-A16

InFlowRate (Flow In): total amount of flux into that cell. Calculated as follows:

```
InFlowRate =
FLOW RIGHT FACE[i,j-1,k] * H(FLOW RIGHT FACE[i,j-1,k])
+ FLOW FRONT FACE[i-1, j, k] * H(FLOW FRONT FACE[i-1, j, k])
+ FLOW LOWER FACE[i,j,k-1] * H(FLOW LOWER FACE[i,j,k-1])
- FLOW RIGHT FACE[i,j,k] * H(-FLOW RIGHT FACE[i,j,k])
- FLOW FRONT FACE[i, j, k] * H(-FLOW FRONT FACE[i, j, k])
- FLOW LOWER FACE[i,j,k] * H(-FLOW LOWER FACE[i,j,k])
```

OutFlowRate (Flow Out): total amount of flux out of that cell. Calculated as follows:

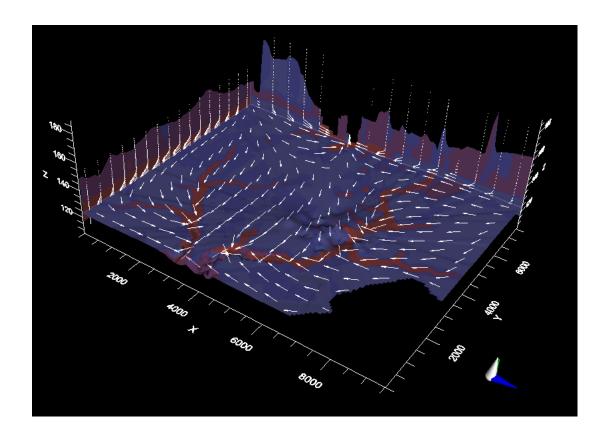
OutFlowRate =
 FLOW RIGHT FACE[i,j,k] * H(FLOW RIGHT FACE[i,j,k])
+ FLOW FRONT FACE[i, j, k] * H(FLOW FRONT FACE[i,j,k])
+ FLOW LOWER FACE[i,j,k] * H(FLOW LOWER FACE[i,j,k])
- FLOW RIGHT FACE[i,j-1,k] * H(-FLOW RIGHT FACE[i,j-1,k])
- FLOW FRONT FACE[i-1,j,k] * H(-FLOW FRONT FACE[i-1,j,k])
- FLOW LOWER FACE[i,j,k-1] * H(-FLOW LOWER FACE[i,j,k-1])

Where H(x) is the Heaviside Step Function; for more details on this function, see: <u>http://mathworld.wolfram.com/HeavisideStepFunction.html</u>

NetFlowRate = InFlowRate - OutFlowRate

Velocity

At the View Maps step, you can view groundwater velocities in a variety of ways as described in the section on <u>3D Gridded Data Settings</u>. By default, velocity vectors are shown as <u>vectors</u>.



Calculation of Velocities in Visual MODFLOW Flex for Finite Difference Grids

Model velocities are estimated in Visual MODFLOW Flex using a two-step process:

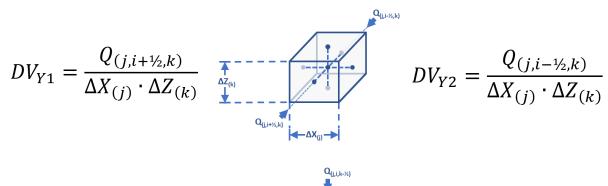
- 1. Estimate inter-cell velocities at each cell face in each component direction (X, Y, and Z)
- 2. Interpolate component velocities to the cell centroid

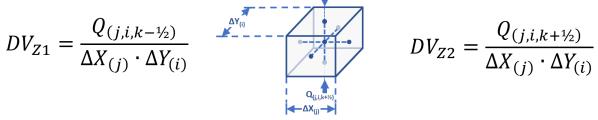
Inter-cell Darcy Velocity and Average Linear Velocity

Inter-cell Darcy velocities (also known as Fluxes) are calculated in Visual MODFLOW Flex using the following equations:

840

$$DV_{X1} = \frac{Q_{(j-\frac{1}{2},i,k)}}{\Delta Y_{(i)} \cdot \Delta Z_{(k)}} \qquad \overset{\Delta Y_{(i)}}{\longrightarrow} \qquad \overset{\Delta Y_{(i)}}{\longrightarrow} \qquad DV_{X2} = \frac{Q_{(j+\frac{1}{2},i,k)}}{\Delta Y_{(i)} \cdot \Delta Z_{(k)}}$$





Inter-cell average linear velocities (V_{ave}) are estimated from the Darcy velocities (DV):

$$V_{ave} = \frac{DV}{\phi_{(i,j,k)}}$$

where:

 $\phi_{(i,j,k)}$ is the calculated value from the model

Component velocities interpolated to the cell centroid

Component velocities are interpolated to the cell centroid by the following equations:

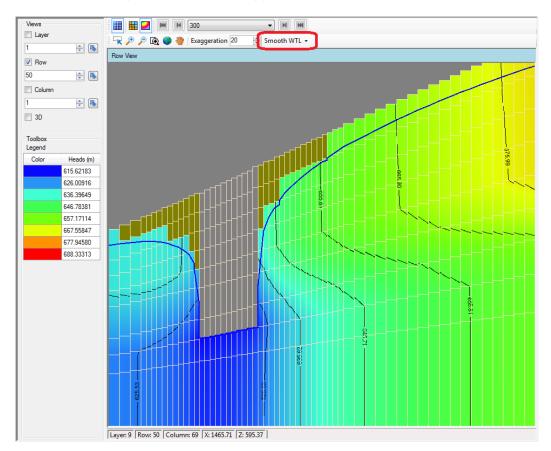
$$V_x = (V_{x1} + V_{x2})/2$$
$$V_y = (V_{y1} + V_{y2})/2$$
$$V_z = (V_{z1} + V_{z2})/2$$

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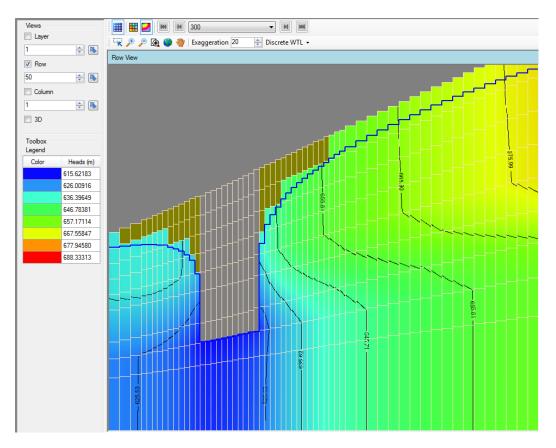
Water Table

The water table is the surface represented by the calculated head in the uppermost active cell in the simulation. In 2D (Layer) and 3D views, the Water Table is displayed as a surface object, and as such has style settings similar to Surfaces (for more details on these options, see <u>Style Settings: Surfaces</u>. In 2D cross-sectional view (by row or column), the water table is drawn as a solid line. On the toolbar above the view, you have an option to control how the line is calculated and displayed.

Smooth WTL (Water Table Line): the line is smoothed (interpolated) between each grid cell. Since the line is interpolated, this is an approximation.



Discrete WTL (Water Table Line): the line is drawn as piecewise constant, with a flat line drawn across each grid cell at the elevation corresponding to the water table. This option better reflects the actual output data and the MODFLOW grid cell geometry.



If your model is Transient, you can adjust the output time as explained above, and the Water table display will update to reflect the new values for that output time.

The Water Table is only calculated for MODFLOW-2000, -2005, -NWT, -SURFACT, and SEAWAT model runs; it is not calculated for MODFLOW-LGR.

Export Water Table

The water table data can also be exported to .CSV file for further post-processing. Rightclick on Water Table from the Model Explorer and select "Export..."

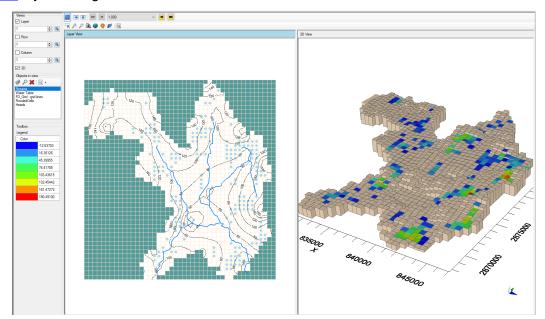
The format of this file is as follows:

- x (x-coordinate at center of cell)
- y (y-coordinate at center of cell)
- ztop (elevation of the top of layer 1; this can be used to calculate depth to water table)
- row
- column
- layer
- wt_"time": water table value at the defined MODFLOW time step; for transient models, you will see additional columns for each saved MODFLOW time step.

	А	В	С	D	E	F	G	Н
1	х	У	ztop	row	column	layer	wt_299.9999	
2	-975	-1950	624.95	1	1	1	624.95	
3	-925	-1950	624.95	1	2	1	624.95	
4	-875	-1950	625.53	1	3	1	625.53	
5	-825	-1950	625.53	1	4	1	625.53	
6	-775	-1950	626.14	1	5	1	626.14	
7	-725	-1950	626.14	1	6	1	626.14	
8	-675	-1950	626.53	1	7	1	626.53	
9	-625	-1950	626.86	1	8	1	626.86	
10	-575	-1950	627.37	1	9	1	627.37	
11	-525	-1950	627.72	1	10	1	627.72	
12	-475	-1950	628.08	1	11	1	628.08	
13	-425	-1950	628.45	1	12	1	628.45	

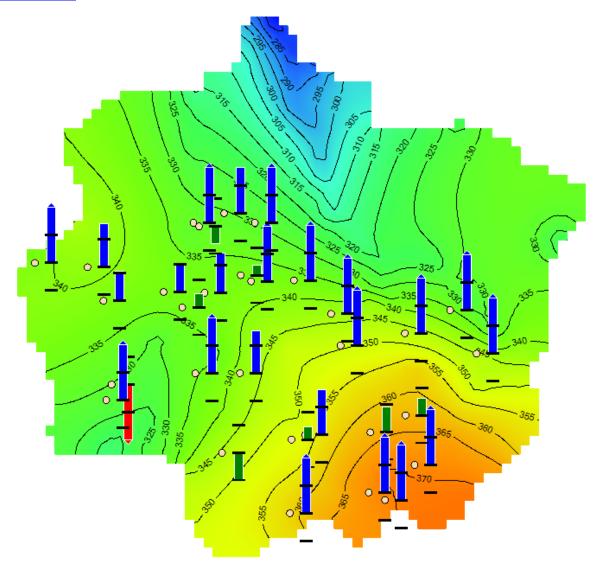
Flooded Cells

Flooded cells are the collection of model cells in the uppermost active layer (i.e. water table cells) with simulated head values greater than the top of the model. These can be visualized as points or cell polygons in 2D and 3D views as a solid color (default is light blue), or using a color ramp based on the depth of flooding (i.e. the difference between the simulated head and the top of the model). Flooded cells have the <u>vertices</u> and <u>time</u> style settings in both the 2D and 3D views at the View Maps workflow step. The 3D view also supports the <u>cells</u> style settings.



Residuals

If your model included observations, you can view residuals relative to a target residual as error bars with various <u>settings</u> at the View Maps step, as described in the section on <u>3D</u> <u>Gridded Data</u>.



Calculation of Residuals

In Visual MODFLOW Flex, residuals are expressed as the difference between the simulated value and the observed value. For example, the heads residuals are calculated as follows:

$$r = h_{calc} - h_{obs}$$

where:

r is the residual value

 h_{calc} is the model-calculated value

 h_{obs} is the observed value

Give that simulated results rarely coincide exactly with the location and time of given observations, Visual MODFLOW Flex interpolates model-calculated results. The interpolation is a two step process - the simulated values are interpolated spatially based on results from the surrounding grid cells. If the model is transient, the spatial values will be interpolated for the output time step before and after the observation and these two values are linearly interpolated in time. Using observations outside of the simulation time is generally not recommended.

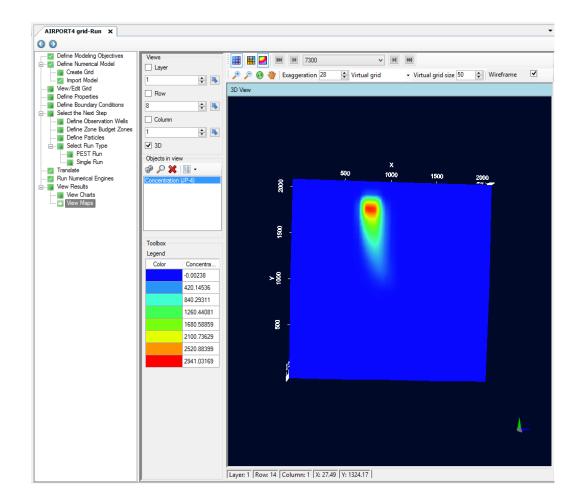
When displayed in Visual MODFLOW Flex, residuals are compared to target residual values which can be set per observation or globally. For more information, please refer to the sections discussing <u>calibration statistics</u> and view <u>settings</u>.

Transport Engine Outputs

Upon successful completion of a transportation engine simulation concentrations and concentration residuals can be visualized at the View Maps step as discussed below.

Concentrations

If you ran a transport simulation (e.g. MT3D-MS, RT3D, or SEAWAT), you will also see output nodes for Concentration (one for each species).

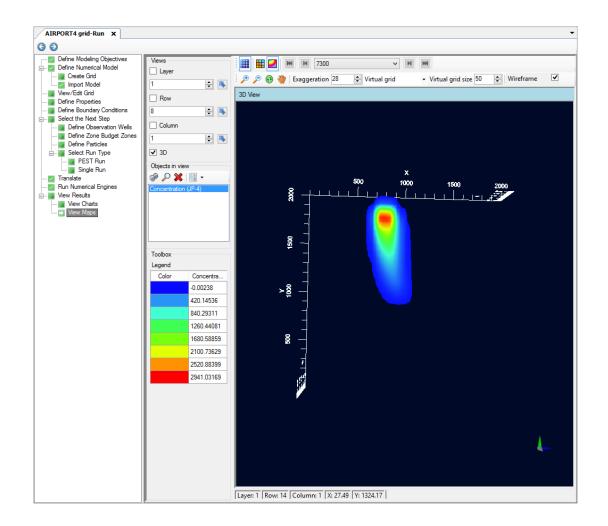


The settings allow you to clip the upper and/or lower levels - for example if we use the Lower Cutoff of 20:

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1	Settings - Concentration (JP-4) – – – ×
General Style Ocells Overtices Overtices Oce Colomap Oceneral Ocors	General ✓ Show Colomap ✓ Use virtual grid Colomap Slice Settings Slice Type Layer
Legend Legend Isolines Isosurfaces Isosurfaces Time	Layer Number (13)
	Fill Settings Transparency 0
	Show Legend Wireframe Use Upper Cutoff: Upper Cut Level 0 ✓ Use Lower Cutoff: Lower Cut Level 20
	Apply <u>Q</u> K <u>C</u> ancel Help

This would result in the following rendering of the concentrations:



The option to use lower and upper cutoffs are available both for Colormap and ThreeSlices display options.

Concentration Residuals

If the transport simulation included concentration observations, you will also output nodes for Concentration residuals (one for each observed species). Similar to residuals for heads, you can view concentration residuals relative to a target residual as error bars with various <u>settings</u>, as described in the section on <u>3D Gridded Data</u>.

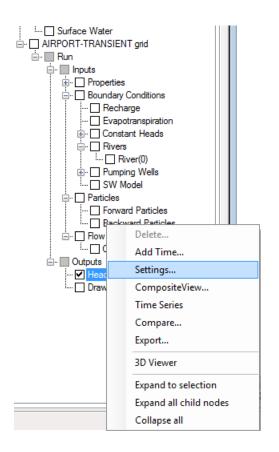
Adjusting Style Settings

The style settings of either the 2D or 3D views can be adjusted (note, each one must be defined independently)

First make the desired property group selected and visible in the Flex Viewer.

Next make the desired 2D viewer active

Then right-click on the desired property group in the tree as shown below and select `Settings`



The 2D Colors and Contour line settings can be adjusted. For more details, see <u>Color and</u> <u>Contour settings</u>

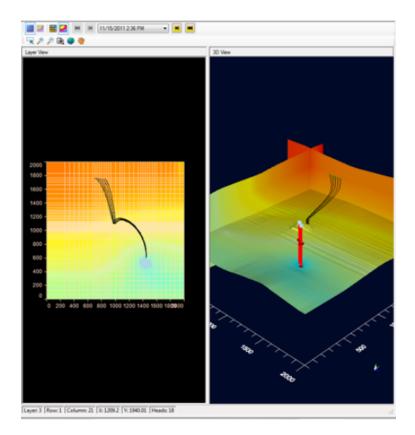
Exporting Outputs.

Outputs can also be exported in a variety of formats. Please see the section on Exporting Files for more details.

10.12.1.1 Pathlines and Time Markers

Visual MODFLOW Flex includes options to adjust the Pathline travel time and time marker for a MODPATH or a MOD-PATH3DU particle track run (using either forward or backward particles).

If you ran a particle tracking simulation, you will see Pathlines appear as a new node (per particle group) in the tree under Output; add a check box beside the Pathlines to display these in the active 2D/3D Viewers.



The pathlines delineate the flow path and travel time of groundwater particles due to advective groundwater flow (as calculated by MODPATH/MOD-PATH3DU). The Pathlines Map is a little different from the other map types because it does not simply represent a "snap-shot" in time. Pathlines represent a historical travel log of the groundwater particles. Forward tracking pathlines are used to predict where groundwater is flowing, and how long it will take to reach a given location if it starts from a known location at a known time. Backward tracking pathlines are used to predict where groundwater at a given location and time is coming from, and how long it took to get there.

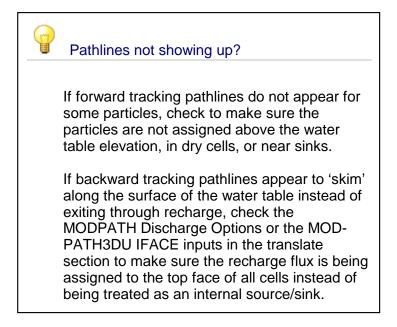
The "Pathlines Options" can be launched by right-clicking on Pathlines from the model explorer, and selecting "Pathline Options". The following window will appear (note that forward and backward pathlines can each have their own settings defined in the Options window.

Pathline Options -	×	
Tracking time		
 Steady state 		
 Travel time (day) 		
0		
Tracking markers		
Visible		
 Regular intervals (day) 		
365		
O Custom intervals		
Time		
•		
Apply OK	Cancel	

The Tracking time frame is used to select either Steady state pathlines (for all times), or to specify a maximum Travel time for all pathlines.

The Time markers frame is used to hide/show the pathline time markers (using the Visible checkbox), and to select the time intervals for each time marker. The Time markers can be plotted at Regular time intervals, or at Custom intervals selected by the user.

The pathline color and thickness can be adjusted in the Settings window; right click on the Pathlines object from the model explorer and select Settings.

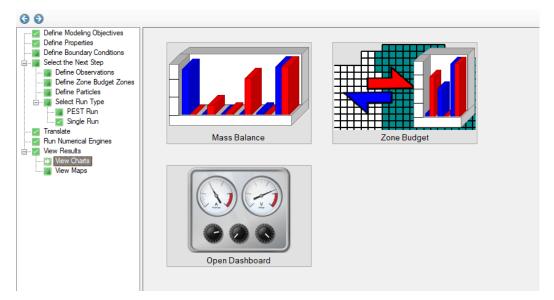


Export

Pathline and time markers can be exported to shapefiles for further analysis; right-click on the Forward or Backward Pathlines on the model explorer, and choose Export. A points shapefile will be created for the time markers, and a polyline shapefile will be created for the pathlines. The exported files will utilize the pathline options you have currently defined in the view for the tracking time and time marker frequency.

10.12.2 View Charts

In Visual MODFLOW Flex, upon completing a successful model run, you can view several different types of charts to review your results and to facilitate model calibration.



Calibration Dashboard

The <u>Calibration Dashboard</u> is multi-component tabulation and charting view that is contained in its own tab. The dashboard consists of:

- a **table** of observations and associated modeling results that can be dynamically filtered and sorted,
- a **statistics panel** that dynamically calculates various calibration-related <u>statistics</u> of data visible in the table and in the charts
- charting area that can contain one or more of the following chart types:
 - **Calc. vs obs. chart**: scatter plot comparing calculated values (y-axis) versus corresponding observations (x-axis)
 - Time Series chart: line series plot of simulated results over and observed values vs time

Mass Balance

The <u>Mass Balance Charts</u> include a set of charts that present data from the mass balance outputs from the flow engine listing file:

- **Percent Discrepancy** plots the temporal changes in the Flow Mass Balance (total flow IN minus total flow OUT) expressed as a percentage of the total flow.
- **IN OUT** plots the temporal change in the Flow Mass Balance (total flow IN minus the total flow OUT).
- **Time Series** plots the temporal flows IN and OUT of the system through the individual sources and sinks (flow boundary conditions and storage).
- **Time Step** plots a bar chart of the flow IN to the system and the flow OUT of the system through the individual sources and sinks (flow boundary conditions and storage) for selected Output Times.

Note: this option is not available for unstructured grids (MODFLOW-USG) runs; however, you can obtain the same results by using ZoneBudget with a single zone.

Zone Budget

The <u>ZoneBudget Charts</u> include a set of charts that present data from Zone Budget runs:

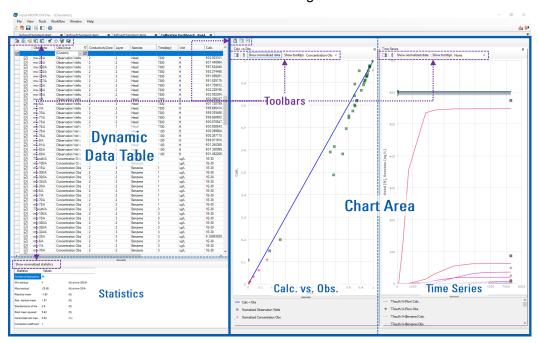
- **Percent Discrepancy** plots the temporal changes in the Flow Mass Balance for the selected zone (total flow IN minus total flow OUT) expressed as a percentage of the total flow in the zone.
- **IN OUT** plots the temporal change in the Flow Mass Balance for the selected zone (total flow IN minus the total flow OUT).
- **Time Series** plots the temporal flows IN and OUT of the selected zone through the individual sources and sinks (flow boundary conditions and storage).
- **Time Steps** plots a bar chart of the flow IN to the system and the flow OUT of the selected zone through the individual sources and sinks (flow boundary conditions and storage) for selected Output Times.

Note: this button is disabled if the run did not include ZoneBudget at the <u>single run</u> (select engines) step.

10.12.2.1 Calibration Dashboard

The calibration dashboard is a standalone multi-component view in Visual MODFLOW Flex that allows you to dynamically filter and plot both observed and simulated values for comparison, calibration, and evaluation purposes.

Layout



The calibration dashboard consists of the following elements:

- a **dynamic data table** of observations and associated modeling results that can be dynamically filtered and sorted,
- a statistics panel that dynamically calculates various calibration-related <u>statistics</u> of data visible in the table and in the charts
- a chart area that can contain one or both of the following chart types:
 - <u>Calc. vs Obs.</u>: scatter plot comparing calculated values (y-axis) versus corresponding observations (x-axis)
 - o *Time Series*: line series plot of simulated results over and observed values vs time
- A set of toolbars in each element that provides related controls

Each of the elements can be resized or hidden/shown using the following controls. Elements can be resized by clicking and dragging the bars that separate them and shown or hidden using the collapse (show/hide) buttons:



Dynamic Data Table

The dynamic data table displays data from all observation groups including observation data, equivalent simulation data, and associated metrics. Following a successful model run, Visual MODFLOW Flex will calculate simulated equivalent values for each <u>observation</u>, extract associated time series data from the simulation for each observation location/observation type, and calculate residuals and normalized values. Data from each observation group is then written to a tab separated variable file (.TSV) with a set number of fields. The TSV file contains two header rows, and is organized in fields (columns) and records (rows).

Headers

The first header row in a TSV file specifies field types:

- SetFilter fields contain descriptive metadata about the observation location that can be used to group or separate data;
- **RangeFilter** fields contain metadata describing the location of the observation in space and time;
- Unit fields contain the unit type for Value fields
- Value fields contain values for observations, calculated values, residuals, target residuals, and normalized values

The second header row in a TSV file specifies field names as described below.

Fields

The following fields are included in each TSV file:

- Visibility: a field with checkboxes that control whether the record is visible (or not) in charts in the chart area (check = visible, unchecked = hidden)
- ObsName: the name of observation well (including well screen id) or gage location [SetFilter]
- **ObsGroup**: the name of the well observation group or gage type [SetFilter]
- X[*unit*]: x-coordinate of the observation location, specified in project length units [RangeFilter]
- Y[*unit*]: y-coordinate of the observation location, specified in project length units [RangeFilter]
- **Z**[*unit*]: z-coordinate of the observation location, specified in project length units [RangeFilter]

- **ConductivityZone**: the conductivity property zone of the observation location [SetFilter]
- Layer: model layer of the observation location [SetFilter]
- **GageType**: type of location measured (e.g. boundary condition type) [SetFilter]
- GageMeasurement: measured parameter (e.g. volumetric flow, head, concentration) [SetFilter]
- Species: measured parameter (e.g. head, solute species) [SetFilter]
- Time[unit]: [RangeFilter]
- Unit: the measurement unit for observed, calculated, residual, and target values (e.g. m, m³/d, mg/L) [Unit]
- Calc.: calculated (simulated) values [Value]
- Obs.: observed values [Value]
- Residual: residual values [Value]
- TargetResidual: specified target residuals [Value]
- NormalizedCalc.: normalized calculated (simulated) values [Value]
- NormalizedObs.: normalized observed values [Value]
- NormalizedResidual: normalized residual values [Value]
- NormalizedTargetResidual: normalized target vales [Value]

One calculated value will be included for each distinct observation that occurs within an active model cell. For observations that do not coincide exactly with model spatial and temporal discretization, calculated outputs are linearly interpolated first in space (based on values from the nearest neighboring cells) and then in time using spatially interpolated values from the times steps that precede and follow the observation. Calculated values without corresponding observations will also be included as separate values for each output time specified in the output control settings for heads and budget-related outputs outputs and for concentrations, as applicable. Normalized values are dimensionless and the calculation of normalized values is described in the calibration statistics discussion. The first row in the table includes controls for filtering the data.

Toolbar

The following controls are available for the tabulated data:



- 🕅 Clear all filters: clears any filters applied to the data
- **Choose Columns**: opens a window that allows you to choose which fields are shown in the table
- Solution Open Data Folder: opens the data subfolder containing the TSV files in the model data folder
- Copy Selected Rows to Clipboard: copies selected table rows to the clipboard for use in other applications

- Copy All to Clipboard: copies all table rows to the clipboard for use in other applications
- Solution Check All: toggles the visibility of all table row data in the charts to visible/on
- Durcheck All: toggles visibility of all table row data in the charts to hidden/off
- W Invert Selection: inverts the selection of all table rows in the charts
- Check/Uncheck selected Rows: checks or unchecks selected table rows in the charts

Filters

The first row in the table is a blank row that allows you to filter the data. When data are filtered, the rows that meet the filter criteria will be shown in the table and charts, and data that do not meet the criteria are hidden. To filter records based on values in a given field, click in the desired field and make use the following controls:



- **Type**: type a value in the field filter entry to filter to show only values that start with the typed value
- **Dropdown**: click the dropdown button to show a list of unique values. Selected values will be shown and all other values will be hidden. The dropdown also includes filters based on the field type:
 - Numeric fields can be filtered using one or more relations to a specified value (equals, does not equal, greater than, greater than or equal, less than, less than or equal, between, or a custom filter)
 - Text fields can be filtered using one or more relations to a specified string (equals, does not equal, begins with, ends with, contains, does not contain, or a custom filter)
- **Clear Filter**: clears any filters on the field

You can clear all filters by using the the clear filter (\mathbb{M}) button at the far left side of the filter row.

Statistics

The statistics panel includes a list of <u>calibration statistics</u> that are commonly used when evaluating model results. These statistics are based on which data rows are shown in the table (i.e. not filtered) and set to visible (i.e. the visibility field is checked on). The following statistics are included:

• Number of observation points

- Minimum (absolute value) residual
- Maximum (absolute value) residual
- Residual mean
- Absolute residual mean
- Standard error of the estimate
- Root Mean Squared
- Normalized Root Mean Squared
- Correlation Coefficient

Each of these statistics is described in the <u>calibration statistics</u> section. The "Show normalized statistics" button allows you to toggle whether the statistics are calculated using actual values or <u>normalized</u> values.

Chart Area

The chart area in the dashboard allows you to display either or both of the charts discussed below.

Toolbar

The following controls are available for the chart area:

1 🔯 🖄

- I Choose Charts: opens a window that allows you to choose which charts are shown
- Symbol Settings: opens the symbology window for the Calc vs. Obs. chart.
- Time Series Settings: opens the symbology window Time Series chart.

Symbology Window

The symbology window allows you to define the symbology of the applicable chart.

Group field ObsGroup Label Symbol Symbol color Riv:VolumetricFlow Circle 128, 0, 51, 255 Observation Wells Observation Wells	
Riv:VolumetricFlow Circle 128, 0, 51, 255	
	lls
Oliver Station Wells	115
Observation Wells Square	
Concentration Obs Diamond Concentration Obs	bs

- **Group Field** (Calc. vs. Obs. only): symbols can be grouped and defined based unique values in one of the <u>setFilter</u> fields in the data table (e.g. observation location name, observation group, conductivity zone, model layer, etc.)
- Label: symbol labels based on the unique values in the grouping field. Note that the Time Series chart are only grouped by observation location (ObsName field)
- **Symbol**: shape of the symbol (circle, square, diamond, pentagon, hexagon, pyramid [triangle], pentagram [star])
- Symbol color: color of the specified symbol (red, green, blue, alpha/opacity)

Calculated versus Observed Calibration Chart (Calc. vs. Obs)

The Calculated vs. Observed Chart consists of a scatter plot representing the comparison between the calculated and observed values shown in the dynamic data table. This graph represents a comparison between the values calculated by the model (Y-axis), and the values observed or measured in the field (X-axis). The situation where all data points intersect the *Calc.=Obs.* line line on the graph represents an ideal calibration scenario, but it is not likely to happen when developing models of real-world sites. If data points appear above the *Calc.=Obs.* line, then the calculated values are larger than the observed values, and the Calibration Residual is positive, indicating that the model is over-predicting. If the data points are under the *Calc.=Obs.* line, then the calculated values are less than the observed values, and the Calibration Residuals are negative, indicating that the model is under-predicting. The chart below indicates the model is generally under-predicting head values.

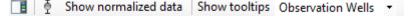


For simulations containing many different observation, types, locations, and times, the quality of the model calibration will likely be quite variable. Therefore, it is important to be able to evaluate the portions of the calibration to evaluate differences between calculated and observed values over different parameter types, spatial locations, and times. You can use the <u>filters</u> and visibility toggles in the <u>dynamic data table</u> to show (or hide) a subset of the data as appropriate. You can also <u>normalize</u> the data to plot different observation types spanning different ranges within a normalized range of 0 to 1.

The chart can optionally include error bars with +/- lengths corresponding to the target residual of each data point. An error bar for a given data point that intersects the *Calc.=Obs.* line indicates that the residuals are within the specified target residual range.

Toolbar

The following controls are available for the Obs. vs. Calc. chart:

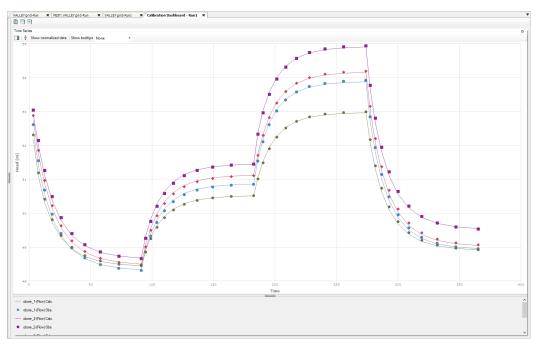


- **I** Toggle Legend Location: toggles whether the legend appears at the bottom of the chart or to the right
- **Toggle Error bars**: toggles whether or not to show error bars. Error bar length is based on the target residual (or normalized target residual if normalized values are shown).
- Show normalized data Show Normalized data: button to toggle whether regular/untransformed data or normalized data are displayed in the chart
- Show tooltips Observation Wells Show tooltips dropdown: allows you to select which series (including a single series, any series, or none) will include tooltips. Tooltips will be displayed for the single data point of the applicable series nearest to the mouse pointer when the pointer is within the chart area.

Time Series Plots

A Time Series graph plots the value of one or more selected variables over time. In groundwater flow and contaminant transport modeling, time-series graphs are used to evaluate and compare temporal trends in the calculated heads, concentrations, flows, or other observations at selected observation wells or gage points. In the Calibration Dashboard Time Series chart, observed values are plotted as discrete points, while corresponding simulated values are plotted as connected lines with same color. The situation where the lines representing simulated data intersect their corresponding observation data points represents an ideal calibration scenario, but it is not likely to happen when developing models of real-world sites. If data points appear above the corresponding simulated result line, then the calculated values are smaller than the observed values, and the calibration residual is negative, indicating that the model is under-predicting the parameter at that location and time. Conversely, if the data points are below the

corresponding simulated result line, then the calculated values are greater than the observed values, and the calibration residuals are positive, indicating that the model is over-predicting. The chart below is based on an exercise using PEST calibration and indicates that model results match observed values well.



For simulations containing many observations of different types, locations, and times, the quality of the model calibration will likely be quite variable and data may not fit neatly on the plot. Therefore, it is important to be able to visualize various subsets of the data to evaluate time series data of interest. You can use the <u>filters</u> and visibility toggles in the <u>dynamic data</u> table to show (or hide) desired subsets of the data. You can also <u>normalize</u> the data to plot different observation types spanning different ranges within a normalized range of 0 to 1.

The chart can optionally include error bars with +/- lengths corresponding to the target residual of each data point. An error bar for a given observation data point that intersects the simulation line indicates that the residuals are within the specified target residual range.

Toolbar

The following controls are available for the Time Series chart:

📑 🖣 Show normalized data Show tooltips Observation Wells 🝷

- **I** Toggle Legend Location: toggles whether the legend appears at the bottom of the chart or to the right
- Toggle Error bars: toggles whether or not to show error bars. Error bar length is based on the target residual (or normalized target residual if normalized values are shown).

- Show normalized data Show Normalized data: button to toggle whether regular/untransformed data or normalized data are displayed in the chart
- Show tooltips Observation Wells Show tooltips dropdown: allows you to select which series (including a single series, any series, or none) will include tooltips. Tooltips will be displayed for the single data point of the applicable series nearest to the mouse pointer when the pointer is within the chart area.

10.12.2.1.1 Calibration Statistics

Calibration Statistics are reported in the footer of the Calibration Plots window when the Calculated vs. Observed Scatter Graph is displayed. These statistics are calculated using the assumption that the calibration residuals are normally distributed. The individual statistics are described below:

Calibration Metrics

The following calibration statistical metric values are calculated by Visual MODFLOW Flex and presented in the Model Dashboard. All metrics are based on the data visible in the table and charts (i.e. not filtered and checked as visible):

Calibration Residual

The calibration residual (R_i) is defined as the difference between the calculated results (X_{cal}) and the observed results (X_{obs}) at selected data points ($i = 1 \rightarrow n$) as shown in the following equation:

$$R_i = X_{cal} - X_{obs}$$

where:

 X_{cal} is the calculated value from the model

 X_{obs} is the measured/observed value

The absolute value maximum and minimum residuals at the selected observation points are also reported. When calculating residuals, it is important to compare values at the same location and point in time. Since observed values and calulated values from model simulations do not always perfectly coincide, when calculating residuals, Visual MODFLOW Flex bi-linearly interpolates the calculated values in space to the location of the observation within the given model layer and then linearly interpolates these values in time to match the time of the observation. Calculated values are <u>not</u> interpolated between layers. As such, groundwater models should ideally be designed so that the gaps in space and time between

observations and corresponding model outputs are relatively small to minimize inaccuracies due to interpolation.

Residual Mean

The residual mean (\overline{R}) is a measure of the average residual value defined by the equation:

$$\bar{R} = \frac{1}{n} \sum_{i=1}^{n} R_i$$

where:

n is the number of observations

 R_i is the ith residual

Please Note: there may be cases where over-calculated and under-calculated values will negate each other, and produce a value of the residual mean close to zero. This can lead to false interpretation of the model calibration – the residual mean should never be used by itself as a measure of the fit between the simulated results and the observed data.

Absolute Residual Mean

The absolute residual mean $(|\bar{R}|)$ is similar to the residual mean except that it is a measure of the average absolute residual value defined by the equation:

$$|\bar{R}| = \frac{1}{n} \sum_{i=1}^{n} |R_i|$$
where:

n is the number of observations

 R_i is the ith residual

The absolute residual mean measures the average *magnitude* of the Residuals, and therefore provides a better indication of calibration than the Residual Mean.

Standard Error of the Estimate

The standard error of the estimate (*SEE*) is a measure of the variability of the residual around the expected residual value, and is expressed by the following equation:

$$SEE = \sqrt{\frac{\frac{1}{n-1}\sum_{i=1}^{n} \left(R_i - \bar{R}\right)^2}{n}}$$

where:

n is the number of observations

 R_i is the ith residual

 \bar{R} is the mean residual (described above)

Root Mean Squared

The Root Mean Squared error (*RMS*) is a measure of the variance of the model residuals and is defined by the following equation:

$$RMS = \sqrt{\frac{1}{n} \sum_{i=1}^{n} R_i^2}$$

where:

n is the number of observations

 R_i is the ith residual

Normalized Root Mean Squared

The Normalized Root Mean Squared (*NRMS*) is the RMS divided by the maximum difference in the observed head values, and is expressed by the following equation:

$$NRMS = \frac{RMS}{(X_{obs})_{max} - (X_{obs})_{min}} \cdot 100\%$$

where:

RMS is the Root Mean Square error (described above)

 X_{obs} is the measured/observed value

The NRMS is expressed as a percentage, and is a more representative measure of the fit than the standard RMS, as it accounts for the scale of the potential range of data values. For example, an RMS value of 1.5 will indicate a poor calibration for a model with a range of observed values between 10 and 20, but it will indicate an excellent calibration for a model with a range of observed values between 100 and 200. The NRMS value for the first model would be 15%, while the NRMS for the second model would be 1.5%. The NRMS values clearly indicate the second model provides a better fit between the calculated and observed values.

Correlation Coefficient

The Correlation Coefficient (*Cor*) is calculated as the covariance (*Cov*) between the calculated results (X_{cal}) and the observed results (X_{obs}) at selected data points divided by the product of their standard deviations. The correlation coefficient is calculated using the following equation:

$$Cor(X_{cal'}, X_{obs}) = \frac{Cov(X_{cal'}, X_{obs})}{\sigma_{cal} \cdot \sigma_{obs}}$$

where:

 X_{cal} is the calculated value from the model

 X_{obs} is measured/observed value

 σ_{cal} is the standard deviation of the calculated values from the model

 σ_{obs} is the standard deviation of the measured/observed values

Cov is the covariance of the calculated and observed values

The covariance is calculated using the following equation:

$$Cov(X_{cal}, X_{obs}) = \frac{1}{n} \sum_{i=1}^{n} (X_{cal} - \bar{X}_{cal}) (X_{obs} - \bar{X}_{obs})$$

where:

 X_{cal} is the calculated value from the model

 X_{obs} is measured/observed value

 $ar{X}_{cal}$ is the mean of the calculated values from the model

 \bar{X}_{obs} is the mean of the measured/observed values

The average values \bar{X}_{cal} and \bar{X}_{obs} are calculated as follows:

$$\bar{X}_{cal} = \frac{1}{n} \sum_{i=1}^{n} X_{cal(i)} , \ \bar{X}_{obs} = \frac{1}{n} \sum_{i=1}^{n} X_{obs(i)}$$

where:

n is the number of observations

 X_{cal} is the calculated value from the model

 X_{obs} is measured/observed value

The standard deviations σ_{cal} and σ_{obs} are calculated as follows:

$$\sigma_{cal} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} \left(X_{cal(i)} - \bar{X}_{cal} \right)^2}, \quad \sigma_{obs} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} \left(X_{obs(i)} - \bar{X}_{obs} \right)^2}$$

where:

n is the number of observations

 X_{cal} is the calculated value from the model

 X_{obs} is measured/observed value

 \bar{X}_{cal} is the mean of the calculated values from the model

 \bar{X}_{obs} is the mean of the measured/observed values

Correlation coefficients range in value from -1.0 to 1.0 and determine whether two ranges of data move together – that is, whether large values of one data set are associated with large values of the other data set (positive correlation), whether small values of one data set are associated with large values of the other data set (negative correlation), or whether values in both sets are unrelated (correlation near zero).

Normalized Values

Visual MODFLOW Flex allows you to normalize (rescale) observed and simulated data values so that different observation/measurement types spanning different orders of magnitude can be simultaneously compared. Values are normalized to the range of values (ΔX_G) within each observation group:

$$\Delta X_G = X_G^{max} - X_G^{min}$$
$$X_G^{max} = max(X_{obs}, X_{cal})$$
$$X_G^{min} = min(X_{obs}, X_{cal})$$

where:

 ΔX is the range of (observed or calculated) values

 X_{G}^{max} is the maximum (observed or calculated) value in the observation group

 X_{G}^{min} is the minimum (observed or calculated) value in the observation group

 X_{obs} is the measured/observed value of the current observation/measurement group

 X_{cal} is the calculated/simulated value of the current observation/measurement group

The scale (κ_G) and translation (λ_G) factors for normalization are based on the range of values and adjusted to avoid division by zero:

$$\kappa_{G} = \begin{vmatrix} \Delta X_{G} > 0 & : & \frac{1}{\Delta X_{G}} \\ \Delta X_{G} = 0, X_{G}^{max} \neq 0 & : & \frac{1}{|X_{G}^{max}|} \\ \Delta X_{G} = 0, X_{G}^{max} = 0 & : & 1 \end{vmatrix}$$

$\lambda_G =$	observed calculated	:	$X_G^{min} \ X_G^{min}$
	residual target residual	:	0 0

Observed and calculated values are translated and scaled, while residuals and target residuals are just scaled:

$$X'_{i} = \kappa_{G}(X_{i} - \lambda_{G})$$
$$r'_{i} = \kappa_{G}(X_{i})$$

where:

 X'_{i} is the ith normalized observed or calculated value in the observation group

 r'_i is the ith normalized residual or target residual

In Visual MODFLOW Flex, the values, whether observed or calculated (simulated) are normalized/rescaled using both observed and calculated values so that the rescaling transformations are consistent and linear and fall within a range of 0 to 1.

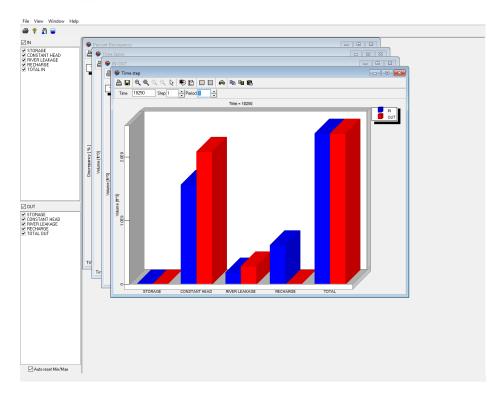
10.12.2.2 Mass Balance Charts

The finite difference formulation of the groundwater flow equation is based on conservation of mass, such that the mass of water entering the system through various sources should equal the mass of water leaving the system through the various sinks. The Mass Balance Graphs provide graphical representations of the mass of water (represented as volume, for MODFLOW models on the assumption of the constant density of water in the simulation domains) entering and leaving the system through the various sources and sinks.

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The Flow Mass Balance Graphs plot the volume and rates of water entering and leaving the system through the flow boundary conditions, and from aquifer storage at the end of each stress period.

To plot the Flow Mass Balance Graphs, select the View Charts workflow step, click the Mass Balance Button on the upper left corner of the Chart view, and a Mass Balance: MODFLOW window will appear as shown below:



There are four different Flow Mass Balance Graphs:

- **Percent Discrepancy** plots the temporal changes in the Flow Mass Balance (total flow IN minus total flow OUT) expressed as a percentage of the total flow.
- **IN OUT** plots the temporal change in the Flow Mass Balance (total flow IN minus the total flow OUT).
- **Time Series** plots the temporal flows IN and OUT of the system through the individual sources and sinks (flow boundary conditions and storage).
- **Time Step** plots a bar chart of the flow IN to the system and the flow OUT of the system through the individual sources and sinks (flow boundary conditions and storage) for selected Output Times.

Note: With both the Time Step and the Time Series graphs, it is important to remember that these graphs present the cumulative volume at a point in time, and not the volumetric loading rate at a point in time.

As mentioned above, the Flow Mass Balance Graphs can be used to plot the flow volume or flow rates of water coming IN and going OUT of the system. By default, the Mass Balance: MODFLOW window plots the flow volume mass balance.

Use the View option in the top menu bar to select either Rates or Volume options, or click

the Cumulative volume (🗧) or Rate (🖺) icon in the toolbar.

Sources and Sinks

On the left-hand side of the Mass Balance: MODFLOW window is a list of all potential sources and sinks for the current flow model (boundary conditions not included in the model will not be listed). These sources and sinks are included in both the IN list and the OUT list. The IN list contains a summary of the flow coming into the system from each individual source term, while the OUT list contains a summary of the flow going out of the system through each individual sink term.

These controls can be used to add or remove the individual source and sink terms from either the Time Series graph or the Time step graph.

The Percent Discrepancy graph and the IN-OUT graph consider only the total flow into and out-of the entire system as a whole. As a result, the settings for the individual IN and OUT terms do not influence the results and appearance of these graphs.

Arranging the Graphs

Each of the Flow Mass Balance Graphs can be maximized to occupy the entire Mass Balance window by clicking the maximize button in the top right-hand corner of each graph window.

Alternately, the graphs can be tiled in the Mass Balance window by selecting Window/Tile from the top menu bar.

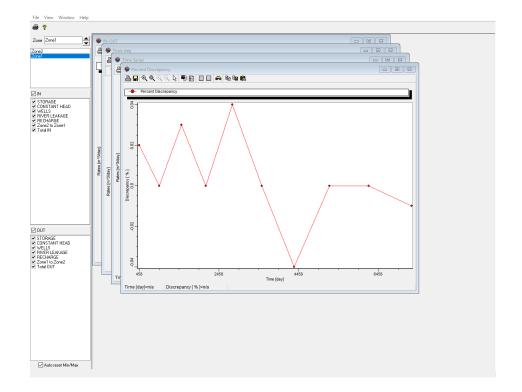
10.12.2.3 ZoneBudget Charts

ZoneBudget is a program developed by the U.S. Geological Survey to calculate water budgets for user-defined zones in the model. The user-defined ZoneBudget zones are created during the Define ZoneBudget Zones step (<u>finite difference</u> or <u>unstructured</u>) workflow step. The Zone Budget program calculates the flow mass balance for each user-defined zone.

Flow Zone Budget Graphs

The Flow Zone Budget Graphs plot the flow rates of water entering and leaving the userdefined zones through the flow boundary conditions, from aquifer storage, and through other user-defined zones.

To plot the Zone Budget Graphs, select the View Charts workflow step, click the Zone Budget Button on the upper left corner of the Chart view, and a Zone Budget: MODFLOW window will appear as shown below:



There are four different Flow Zone Budget Graphs:

- **Percent Discrepancy** plots the temporal changes in the Flow Mass Balance for the selected zone (total flow IN minus total flow OUT) expressed as a percentage of the total flow in the zone.
- **IN OUT** plots the temporal change in the Flow Mass Balance for the selected zone (total flow IN minus the total flow OUT).
- **Time Series** plots the temporal flows IN and OUT of the selected zone through the individual sources and sinks (flow boundary conditions and storage).
- **Time Steps** plots a bar chart of the flow IN to the system and the flow OUT of the selected zone through the individual sources and sinks (flow boundary conditions and storage) for selected Output Times.

Please Note: With both the Time Steps and the Time Series graphs, it is important to remember that these graphs present the rate(s) at a point (or points) in time, and not the cumulative volume at a point in time.

Controls

On the left-hand side of the Zone Budget: MODFLOW window is a list of the Zone Budget zones available for the current model. The Zone Budget graphs described above will display the Zone Budget data for the selected Zone Budget zone.

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The Zone List Box Control

The Zone Control indicates the current Zone for the active charts and the list box below shows all available ZoneBudget zones in the model. Clicking directly on a Zone in the list will switch to that Zone.

The IN/OUT List Box Controls

The IN list contains each of the possible source terms which may contribute flow to the selected Zone Budget zone, while the OUT list contains each of the possible sink terms which may divert flow out of the selected Zone Budget zone.

The checkboxes beside each term can be used to add or remove the individual source and sink terms from either the Time Series graph or the Time step graph.

The group checkboxes will add or remove the entire IN/OUT group.

The Percent Discrepancy graph and the IN-OUT graph consider only the total flow into and out-of the entire system as a whole. As a result, the settings for the individual IN and OUT terms do not influence the results and appearance of these graphs.

Note: By convention, Zone Budget considers mass balance from the perspective of the groundwater system. For example, the IN term for River Leakage represents the river leakage INTO the groundwater system.

Arranging the Graphs

Each of the graphs can be maximized to occupy the entire Zone Budget window by clicking the maximize button in the top right-hand corner of each graph window. Alternately, the graphs can be tiled in the Zone Budget window by selecting Window/Tile from the top menu bar.

10.12.3 Compare Heads and Drawdown

Visual MODFLOW Flex allows you to compare Heads, Drawdowns, or Concentrations between several model runs. This is useful to determining differences in pre and post pumping heads or comparing impacts to results when adjusting property or boundary condition parameters.

Comparing Heads

Follow the steps below:

• Right-click on the Heads node of any model run, and select the "Compare" option. The following dialog will appear

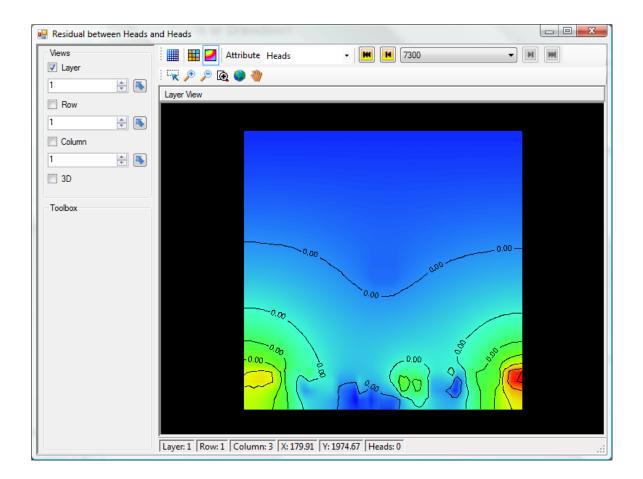
Compare Heads	
Compare Heads with	
Heads from Numerical Model	
MODFLOW .HDS File	
	OK <u>C</u> ancel

There are two options available:

• Select a Heads from the Output tree from another model run; in this case, click on the

Heads node from another model run, and click on the button to add this to the field

- Select a MODFLOW .HDS file from the hard drive, from another model. Click on the Open folder button and browse to a .HDS file on the hard drive.
- Click OK. A new view will appear. The plot shows the results of subtracting the heads selected specified above <u>from</u> the Heads where you launched the `Compare Heads` option.



Comparing Drawdowns or Concentrations

The same option is available for drawdown and concentrations, following steps similar to those outlined above. Simply launch the 'Compare' context menu option from the Drawdown or from one of the Concentrations nodes on the Output model tree and choose the Drawdown/Concentrations from another model run, or from a results file from the computer. Drawdowns are stored as .DDN files and concentrations are stored as .UCN files with the species index as a prefix. If sorption or a dual domain is included in the model, the sorbed/immobile domain concentration results include "S" in the prefix.

Limitations

The comparison calculation has the following assumptions: Both models must have the same:

- start date (as defined in the Conceptual Model settings),
- spatial coverage (XY extents), and
- angle of rotation

Please Note: when comparing two sets of model results with non-aligned schedules, the comparison will merge the schedules by adding all time steps from both schedules and comparing the most recent values for the displayed time step *without temporal interpolation*. As such, using output schedules that match exactly results in a more precise comparison and should be used where possible.

10.13 Duplicating Models

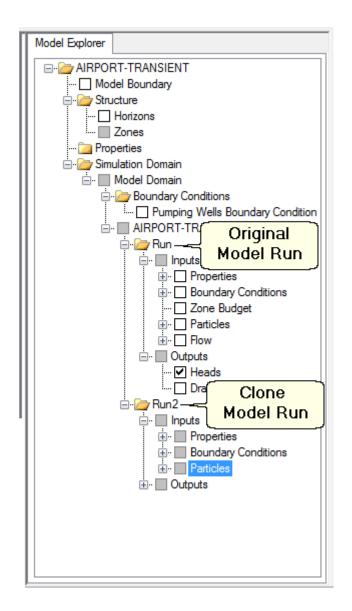
Traditionally, multiple scenarios of a model would be handled by saving the entire project as a new file. This makes it difficult to keep track of various versions of the model and which inputs lead to specific results, etc.

In Visual MODFLOW Flex, a numerical model run can be duplicated or 'cloned' and managed and modified in a single project. This facilitates an iterative approach to modeling by allowing you to adjust a few input parameters, translate and run, and interpret the results. You can also Compare Heads or Drawdown between model runs to other scenarios.

To Clone a numerical model, follow the steps below.

Model Explorer					
AIRPORT-TRANSIEN	Т				
Model Boundary					
🧁 Structure					
Horizons					
Energy En					
Properties					
Simulation Domain					
····· □ Pumping Wells Boundary Condition □·· □ AIRPORT-TRANSIENT grid					
AIRPORT	-TRANSIENT gro				
	Open Related Workflow(s)				
	Clone				
	Settings				
	Delete				
	Expand to selection				
	Expand all child nodes				
	Collapse all				

After this the model tree will be duplicated and added under the selected numerical grid; a new Numerical Model workflow will then load where you can work with this model run clone.



The Workflow and Model Explorer are closely associated; as you progress through a specific numerical model workflow, the items you see in the Flex Viewer originate from the corresponding Run folder on the Model Explorer. For example, if you are working a clone of a model run, eg. Run2, and you are viewing boundary condition cells, you will see these originate from the After this the model tree will be duplicated and added under the selected numerical grid; a new Numerical Model workflow will then load where you can work with this model run clone.

10.14 Exporting Data

Visual MODFLOW Flex allows you to export some raw data and most of the numerical model inputs and outputs to shapefiles for external analysis.

Data Objects

Data ojects in the Data Explorer can be exported to external formats as follows:

- Points, Polygons and Polylines can be exported to shapefiles (*.SHP), or commaseparated values text files (*.CSV)
- Well Objects can be exported to Excel (*.xlsx)
- Surfaces and Horizons exported to comma-separated values text files (*.CSV)
- Surfaces that have been generated based on a uniform grid spacing (i.e. $\Delta X = \Delta Y = constant$) can also be exported to a Surfer ASCII grid files (*.GRD)

To export a data object:

- From the Data Explorer, right-click on the desired data object, and select Export from the pop-up menu.
- A Save As dialog box will display on your screen
- Specify a file Name and Folder location, and the File Type for the exported file, and then click the [Save] button.
- Click the [OK] button from the Export dialog box.

Model Explorer Objects

Exporting to Shapefiles

Export to points or polygon shapefile is currently available for the following:

- Model Inputs:
 - Numerical Grid
 - Properties: Conductivity, Storativity, Initial Heads, Longitudinal Dispersion, Species Parameters, Initial Concentrations, and Bulk Density
 - o Boundary Conditions: Recharge, Evapotranspiration, and UZF
 - Zone Budget Zones
- Model Outputs:
 - \circ Heads
 - o Drawdown
 - Budget
 - Velocity
 - o Concentration: each constituent species must be exported separately

When exporting point shapefiles, one point will be exported for each applicable cell centroid. When exporting polygon shapefiles, one polygon will be exported for each applicable cell.

To export data on the model explorer, right-click on the desired item (eg. Conductivity), and select Export... as shown below.

AIRPORT-TRANSIENT grid				
···· Conduct		Settings		
···· 🗌 Initial He		Composite View		
Boundary Condit		Delete		
		Export		
⊡ Constant He □ □ CH - Up □ □ CH - Lov		3D Viewer		
		Expand to selection		
CH - Lov		•		
⊡. □ Rivers		Expand all child nodes		
🗌 River(0)		Collapse all		
🖃 🔲 Pumping We	Well icles article	s Boundary Condition		

The following dialog will appear; note at the bottom you have the option to choose Points Shapefile or Polygon Shapefile depending on the type of data to be exported.

🐯 Save As				×
	ExportTest	•	€	٩
🎍 Organize 👻 🏢 Views 👻 📑 New Folder				?
Favorite Links	Name	Date modified	Туре	Size
Documents		This folder is e	mpty.	
More »				
Folders 🗸				
Desktop 🔺				
Administrator				
Public				
Computer				
DATA (D:)				
DVD/CD-RW Drive (E:)				
File name: Conductivity.SHP				•
Save as type: ESRI - point shapefile (*.SHP)			-
ESRI - point shapefile (*.SHP				
Hide Folders ESRI - polygon shapfile (*.SH				
Hide Folders			Jave	

Click OK. Depending on the type of data, you may have additional settings. The following options are available for Properties:

😂 Export	x
Select Co-ordinate System:	
World Co-ordinate 🔹	
Add Column Names	
Null Value in Inactive Cells:	
Select Attributes	Select Layers
Select All	Select All
 ✓ Layer ✓ Row ✓ Column ✓ Zones ✓ Kx ✓ Ky ✓ Kz 	V Layer 1 Layer 2 Layer 3
	QK <u>C</u> ancel

Choose which attributes you want to be generated and what layers should be included.

Click OK and the shapefile will be created.

Exporting Output Heads and Concentrations

The following additional options are available for exported output Heads, Concentrations, or the Water table:

🐯 Export	×
Select Co-ordinate System: World Co-ordinate Add Column Names Null Value in Inactive or Dry Cells: 1E+30 -1E+30	Heads at Time Select Heads at All Time 500 666 2000 3000 4000 6000 500
Select Attributes	7300 Select Layers Select All
✓ Layer ✓ Row ✓ Column	Layer 1 Layer 2 Layer 3
	QK <u>C</u> ancel

Choose which attributes you want to be generated and what layers should be included. Note that the Layer options are not available for the Water table.

If your model has transient heads, you have an option to include Heads from multiple times as separate attributes in the shapefile .DBF file. Choose specific times or 'Select Heads at All Times' to include all heads.

A Notation in Shapefile DBFs					
There are some restrictions on attribute names in DBF files; the length is restricted to 10 characters, and certain characters cannot be used, including decimal (.), hyphens (-), and plus sign (+). As such, Visual MODFLOW Flex uses the following notation:					
For transient heads, the attribute name notation is HT (head at time) followed by the time value - an underscore is used in place of a decimal, M is used in place of hyphen, and is used in place of plus.					
For example:					
Output times 1E-5 500.25 9E+7	Notation in DBF file HT_1EM5 HT_500_25 HT_9EP7				

Exporting Output Budget

You are also able to export flow budget data for the model and Boundary Condition cells as a comma separated variable (.CSV) text file. After you have run your model you will find Budget in the Output of the model explorer - right click and select export and the Export fluxes dialog will appear.

Export Budget				_		\times
Save to file name						
Layers	Time Steps		Attributes			
Layer 1 Layer 2 Layer 3 Layer 4 Layer 5 Layer 6	1.0000		XRate YRate ZRate InFlowRa OutFlowR Vells Drains Constant River Lea	Rate Rate Heads		
Export as: Export World Coordinates		\sim	Export Only	Applica	ble Cells	I
	ОК	Cano	el			

880

You must specify the location of the file. You can also select which layer(s), time step(s), and attributes(s) to export. The XRate, YRate, ZRate, InflowRate, OutFlowRate, and NetFlowRate will always be available in the attributes list. While the attributes list will also contains a list of boundary conditions budget terms that are active in the model (in the case shown above the list includes Wells, Drains, Recharge, Constant Heads, and Rivers).

Exporting Contours

Output contour lines can be exported as polyline shapefiles for further analysis and mapping in external applications. To do this, enable the 3D subview to render the contours, then rightclick on the contoured output (e.g. Heads, Drawdown, Water table, Concentrations) and select "Export contours...". A polyline shapefile will be created for the contours as specified in the relevant object settings. You can adjust the contour lines, including adding custom lines, using the <u>ThreeSlices>ContourLine</u> settings in the 3D subview or the <u>ContourLine</u> settings in a 2D subview.

Exporting Particle Pathlines

Pathline and time markers can be exported to shapefiles for further analysis; right-click on the Forward or Backward Pathlines on the model explorer, and choose Export. A points shapefile will be created for the time markers, and a polyline shapefile will be created for the pathlines. The exported files will utilize the pathline options you have currently defined in the view for the tracking time and time marker frequency. See the <u>section</u> on visualizing particle track results for more information.

Exporting to Text Files

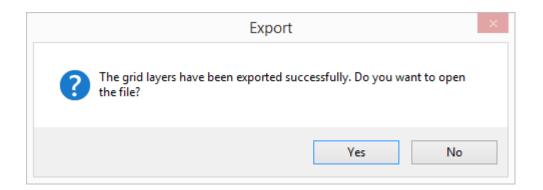
Export to Text-IJK/.CSV files is currently available for the following:

- Model Inputs
 - o Model Layers
 - Boundary Conditions: all, including wells, but excluding recharge, evapotranspiration, and UZF
- Model Outputs
 - \circ Water Table

You can export your Model Layers to .CSV or .TXT by right-clicking on the grid in the Model Explorer and selecting Export Layers...

Then you can provide the location and select if you want .CSV or .TXT.

Once you select Save you will be notified that the layers have been exported and given the option to open the exported file.



The resulting file will contain Layer, Row, Column, X, Y, Z, Top, Bottom, and Thickness information.

	NumericalGrid1.CSV - Notepad -		×
File	Edit Format View Help		
Lay	er,Row,Column,X,Y,Z,Top,Bottom,Thickness		
1,1	,1,67.0382060820452,3950,218.438621095238,1E+31,1E+31,1E+31		
1,1	,2,201.114618246136,3950,218.438621095238,1E+31,1E+31,1E+31		
1,1	,3,335.191030410227,3950,218.438621095238,1E+31,1E+31,1E+31		
1,1	,4,469.267442574318,3950,218.438621095238,1E+31,1E+31,1E+31		
1,1	,5,603.343854738409,3950,218.438621095238,1E+31,1E+31,1E+31		
1,1	,6,737.4202669025,3950,218.438621095238,1E+31,1E+31,1E+31		
1,1	,7,871.496679066591,3950,218.438621095238,1E+31,1E+31,1E+31		
1,1	,8,1005.57309123068,3950,218.438621095238,1E+31,1E+31,1E+31		
1,1	,9,1139.64950339477,3950,231.094340860528,244.325319509128,217.863362211928,26.4619572971998		
1,1	,10,1273.72591555886,3950,231.271354672294,244.536228327017,218.00648101757,26.5297473094472		
1,1	,11,1407.80232772295,3950,231.481505943463,244.781143510826,218.1818683761,26.5992751347257		
1,1	,12,1541.87873988705,3950,231.615064008971,244.989825043005,218.240302974938,26.7495220680675		
1,1	,13,1675.95515205114,3950,231.68932267575,245.207405133924,218.171240217577,27.036164916347		
1,1	,14,1810.03156421523,3950,231.744426689832,245.416690048836,218.072163330828,27.3445267180081		
1,1	,15,1944.10797637932,3950,231.803986279806,245.616854574685,217.991117984927,27.6257365897582		
1,1	16,2078.18438854341,3950,231.771724721802,245.400720761288,218.142728682316,27.257992078972		
1,1	,17,2212.2608007075,3950,231.69888073026,244.915616228694,218.482145231826,26.433470996868		
1,1	,18,2346.33721287159,3950,231.609369320633,244.426470163465,218.792268477801,25.634201685664		
	,19,2480.41362503568,3950,231.485395675686,243.982440279959,218.988351071413,24.9940892085464	Ļ	
	,20,2614.49003719977,3950,231.220609560526,243.545284097587,218.895935023465,24.6493490741223		
	,21,2748.56644936386,3950,231.042425000401,243.339667476867,218.745182523935,24.5944849529324		
	,22,2882.64286152795,3950,230.73646467106,243.025343369822,218.447585972299,24.5777573975235		
	,23,3016.71927369205,3950,230.321709743374,242.63356994394,218.009849542807,24.6237204011324		
	,24,3150.79568585614,3950,229.834323138542,242.248389875795,217.420256401288,24.8281334745064		
	, 25, 3284.87209802023, 3950, 229.414996506131, 241.926414811405, 216.903578200858, 25.022836610547		
	26,3418.94851018432,3950,229.042261194978,241.650905360587,216.433617029369,25.2172883312174	Ļ	
	27,3553.02492234841,3950,228.552829284087,241.092738349848,216.012920218326,25.0798181315215		
	28,3687.1013345125,3950,228.14125406183,240.415084003023,215.867424120637,24.5476598823862		
	,29,3821.17774667659,3950,227.809726963499,239.768970989031,215.850482937967,23.9184880510637		
	,30,3955.25415884068,3950,227.525080170975,239.202238533783,215.847921808167,23.3543167256162		
	,31,4089.33057100477,3950,227.132536845318,238.432836167299,215.832237523336,22.6005986439637		

Boundary conditions can be exported using the same steps described for exporting Model Layers above. Boundary condition data fields will be exported along with the Layer, Row, and Column data fields. Data fields for stress period start and end times will be added if the boundary condition is transient.

11 Numerical Modeling Workflow - Unstructured Grids (MODFLOW-USG)

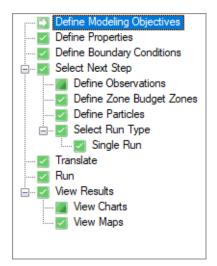
This chapter presents information on editing data in a numerical model workflow for unstructured Voronoi grids (V-Grids) and Quadtree grids (Q-Grids). The numerical models for unstructured grids are generated after you run the Conceptual to Numerical conversion step.



You must have a license of Pro or Premium in order to use the Unstructured Grid numerical workflow in Visual MODFLOW Flex.

The numerical modeling workflow provides the tools for defining, viewing, and editing the numerical model (properties and boundaries assigned to grid cells), creating the model input files, running the MODFLOW-6 or MODFLOW-USG engine, and analyzing the results. The following sections are covered:

- 1. Define Modeling Objectives
- 2. <u>Define Properties</u> (edit parameter values, display in plan, XS, and 3D views)
- 3. <u>Define Boundary Conditions</u> (constant heads, drains, pumping wells, recharge, etc.)
- 4. Select Next Step
 - a. Define Observations
 - b. Define Zone Budget Zones
 - c. <u>Define Particles</u>
 - d. Select Run Type/Single Run
- 5. Translate
- 6. <u>Run</u>
- 7. View Results
 - a. View Charts
 - b. <u>View Maps</u>



For more details on how MODFLOW-USG differs from traditional versions of MODFLOW, please see our <u>website</u>.

For more details on MODFLOW-USG, and the formats for the packages, please see the USGS website.

11.1 Define Modeling Objectives- USG

The first step in the workflow for developing and running numerical models in Visual MODFLOW Flex is to define the modeling objectives. This entails selecting the desired simulation options. The selected combination of flow options (e.g. saturated groundwater flow) and transport options (e.g. reaction and sorption models) will narrow the list of available flow and transport engines and generate associated input variables (including units and default values). The purpose of this step is to develop the necessary inputs required to build the model based on your understanding of the relevant physical processes present within the study area.

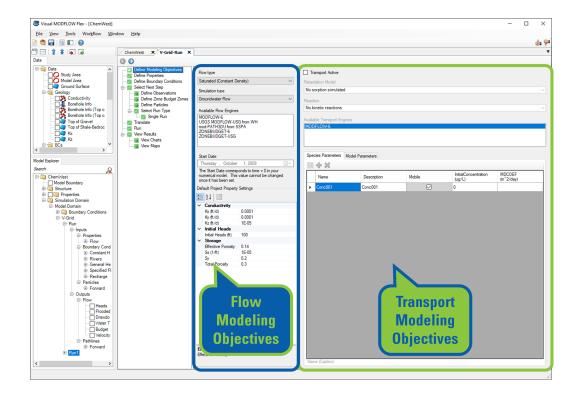
The numerical workflow for unstructured grids supports the following engines:

Flow	Transport	Utilities	
MODFLOW-USG	• <u>not supported</u>	 ZONEBUDGET MOD-PATH3DU¹ 	
MODFLOW-6	MODFLOW-6	• ZONEBUDGET-6	

Engines supported in Visual MODFLOW Flex

Notes:

1 - MOD-PATH3DU is a particle-tracking algorithm developed by a collaboration between S.S. Papadopulos & Associates (SSPA) and the University of Waterloo. It is not installed directly with Visual MODFLOW Flex and must be downloaded and installed separately from the <u>mod-PATH3DU</u> website.



Understanding Default Values at the Modeling Objectives Step

Values set at the Define Modeling Objectives workflow step are used by Visual MODFLOW Flex to populate the applicable arrays for the flow and transport model consistent with the modeling objectives upon reaching the Define Properties Step for the first time. Constant values (discussed below) are the exception to this and are discussed below.

Once the applicable arrays have been created in the Model Explorer, changes to the default values at the Define Modeling Objectives will not be reflected in the Flow Model. To reset values for a group of properties (e.g. Conductivity, Storage parameters, or initial heads) delete the relevant node from the Model Explorer Tree, update the default value at the Modeling Objectives step and proceed to the Define Property Zones step to regenerate the deleted arrays with the updated defaults.

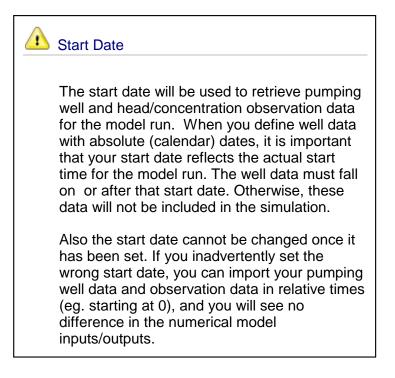
Flow Objectives

Under the left panel of Define Modeling Objectives, you can specify a Start Date for the project. Pumping well data and calibration data (head and concentration observation wells) are entered and save as absolute (calendar) dates. Therefore, it is important to choose a relevant start date at this step that coincides with the start time of your simulation.

Flow and Simulation Type

Currently, only saturated groundwater flow can be simulated using the unstructured grid numerical modeling workflow.

Under Property Settings, you can modify the default flow parameters.



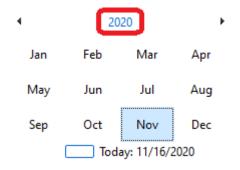
Start Date

Visual MODFLOW Flex uses a standard Windows date picker; a few tips are shown below on how to use this. For example to set a model start date of January 1, 2000.

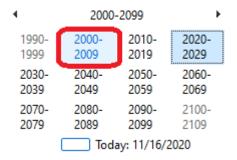
- Click on the button shown below, to load the Windows date picker.
- The standard Windows calendar will appear. Click on the month in the header (as shown below):

•	1	Nove	ember	2020		×
Sun	Mon	Tue	Wed	Thu	Fri	Sat
25	26	27	28	29	30	31
1	2	3	4	5	6	7
8	9	10	11	12	13	14
15	16	17	18	19	20	21
22	23	24	25	26	27	28
29	30	1	2	3	4	5
		1	loday:	11/16/	/2020	

• All months for the current year will appear as shown below. Click on the year in the header:



• A range of years will then appear as shown below. Click on the range of years in the header:

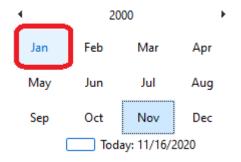


A list of years for the previous decade will appear. You can then use the < or > buttons to change the year.

• Once you have reached the desired year (2000 for this example), select this on the calendar as shown below:



 A list of months will then appear for that year. Select January for this example, as shown below.



• Finally, select "1" from the calendar as shown below:

4		•				
Sun	Mon	Tue	Wed	Thu	Fri	Sat
26	27	28	29	30	31	1
2	3	4	5	6	7	8
9	10	11	12	13	14	15
16	17	18	19	20	21	22
23	24	25	26	27	28	29
30	31	1	2	3	4	5
		I	foday:	11/16/	/2020	

The selected date will then appear for the Start Date.

Transport Objectives

The transport objectives are defined on the right panel of the Define Modeling Objectives window. When you select the "Transport Active" check box at the top of the screen, then the options can be defined as explained and shown below.

Retardation Model

Transport engine retardation model options are currently supported in Visual MODFLOW Flex as follows:

Description	MF- USG	MF-6
No Sorption		
Linear sorption (equilibrium controlled)		V
Freundlich (equilibrium-controlled)		
Langmuir (equilibrium-controlled)		\checkmark
Dual-domain mass-transfer without sorption		
Dual-domain mass-transfer with linear sorption in mobile domain		V
Dual-Domain with Complex Sorption Options		
Triple-Domain with Complex Sorption Options		\checkmark
Quadruple-Domain with Complex Sorption Options		V
Dual-domain mass-transfer (with the same linear sorption in mobile and immobile domains)		
Dual-domain mass-transfer (with different linear sorption in mobile and immobile domains)		V

Reaction

Transport engine reaction model options are currently supported in Visual MODFLOW Flex as follows:

Description	MF- USG	MF-6
No kinetic reactions		V
First-order irreversible decay		V
Zeroth-order irreversible decay		
Complex Model Reactions ¹		M

Notes:

1 - Complex Reactions available for MODFLOW-6 allow for different reaction models (no kinetic reactions, first-order, and zero order decay) to be independently specified for each species and for each (mobile/immobile domain) in the aqueous and sorbed phases. Complex model reactions are only compatible with the three available complex sorption options (i.e. dual-domain, triple-domain, and quadruple-domain).

The selections you make for Sorption and Reaction options will determine what parameters you need to define for your model. Default values can be defined in the "Species Parameters" and "Model Parameter" tabs. After the model is created, you can define additional zonation for Transport Properties at the "Define Properties" step. Detailed information regarding these parameters can be found in the MODFOW-USG and MODFLOW-6 User Manuals (please see the <u>references</u> section).

The New Species and Delete Species buttons allow you to add and remove species to your Transport simulation. This option is available only for certain transport engines.

When you Species Parameter tab is selected, use the add button ($^{+}$) to add a new species, or use the remove button ($^{\times}$) to remove the selected species.

Please Note: the remove button will remove the *last* species in the list.

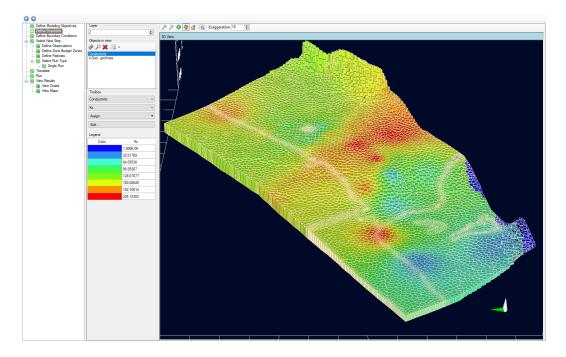
The model parameters window is shown below. For more information, see the individual sections describing <u>Species Parameters</u> and <u>Model Parameters</u>.

an	dation Model						
ua	druple Domain W	Vith Complex Sorption					
act	tion						
_	t-order irreversib	le decay					
	able Transport Eng DFLOW-6	gines					
ΟL							
ipe	cies Parameters	Model Parameters					
ipe	cies Parameters Name	Model Parameters Designation	Description	Value		Units	SpatiallyVariable
ipe •	1		Description How should reacti	Value By cell	~	Units	SpatiallyVariable
	Name				~	Units kg/m^3	SpatiallyVariable
	Name IRCTOP	Designation	How should reacti	By cell	~		SpatiallyVariable
	Name IRCTOP RHOB	Designation Bulk density	How should reacti Dry bulk density of	By cell 1700	~	kg/m^3	SpatiallyVariable
	Name IRCTOP RHOB RhobIm	Bulk density of th	How should reacti Dry bulk density of Dry bulk density of	By cell 1700 1700.0	~	kg/m^3 kg/m^3	
	Name IRCTOP RHOB RhobIm Rhobim2	Designation Bulk density Bulk density of th Immobile Bulk De	How should reacti Dry bulk density of Dry bulk density of Dry bulk density of	By cell 1700 1700.0 1700	~	kg/m^3 kg/m^3 kg/m^3	
	Name IRCTOP RHOB RhobIm Rhobim2 Rhobim3	Bulk density Bulk density of th Immobile Bulk De Immobile Bulk De	How should reacti Dry bulk density of Dry bulk density of Dry bulk density of Dry bulk density of	By cell 1700 1700.0 1700 1700	~	kg/m^3 kg/m^3 kg/m^3	

When you are finished, click 💟 (Next Step) to proceed.

11.2 Define Properties

At this step, you can edit the flow (and transport) properties for the model. You can also adjust the view/style setting of properties or export the properties.



You can assign properties while viewing either by Layer, Row, or Column; however you cannot edit properties when the 3D subview is active.

Under the Toolbox, use the combo box to select from the available property groups:

- Flow Parameters
 - □ <u>Conductivity</u>: includes horizontal conductivity in the X direction (Kx), in the Ydirection (Ky), and vertical conductivity (Kz)
 - □ <u>Storage</u>: includes Specific Storage (Ss), Specific Yield (Sy), Total Porosity (Tp), and Effective Porosity (Ep)
 - □ Initial Heads

When transport is included with your model, the following additional property groups may be included:

Transport Parameters

 Initial Concentration Group - one node for each Species
 Species Parameters Group(s) - one or more node for each Species
 Model Parameters Group(s)
 Dispersion

Please Note: the number of Species Parameters and Model Parameters (if any) will depend on what Sorption and Reaction options you have defined in the <u>Define</u> <u>Modeling Objectives</u> step. Please also refer to the <u>Theory</u> section.

For each parameter group, you can choose to render by Zones or by a selected attribute (for example the Conductivity group includes attributes for Kx, Ky, and Kz). Based on your selection, the color rendering in the views will change.

Edit

Select the Edit button to edit Property zone values after they have been assigned and the Edit property dialog is launched. Here you can select the zone and then you will have the ability to edit any of the cells that are part of the zone.

lit Cells Script								
Zones Conductivity 🙀 Calculation 🗸 🔛 💷								
Zone	Cell	∀ Kx (ft/d)	∀ Ky (ft/d)	Ƴ Kz (ft/d)	7			
1	1351	1E-06	1E-06	1E-07				
2	1362	1E-06	1E-06	1E-05				
3	1363	1E-06	1E-06	1E-05				
5	1365	1E-06	1E-06	1E-05				
6	1368	1E-06	1E-06	1E-05				
	1370	1E-06	1E-06	1E-05				
	1371	1E-06	1E-06	1E-05				
	1374	1E-06	1E-06	1E-05				
	1381	1E-06	1E-06	1E-05				
	1386	1E-06	1E-06	1E-05				
	1388	1E-06	1E-06	1E-05				
	1390	1E-06	1E-06	1E-05				
	1391	1E-06	1E-06	1E-05				
	1398	1E-06	1E-06	1E-05				
	1405	1E-06	1E-06	1E-05				
	1406	1E-06	1E-06	1E-05				
	1407	1E-06	1E-06	1E-05				

The following buttons are available to assist with your edits:

\sqrt{x}	Expression Builder
	Assign to current cell
	Assign to column
	Apply to selected cells

The Expression Builder, which can be accessed by clicking the \sqrt{x} button, helps you to construct expressions that can include variables and mathematical functions to update property values.

Also available is the Script tab. If preferred, you can make your edits by using the Script option. On this tab you will find the script for any edits you make on the Edit Cells tab allowing you to learn the script language. You can then use the script to "replay" the same edits again.

Adjusting Style Settings

Most of the display settings for the flow or transport properties of a 3D unstructured grid are the same as what are available a 3D structured (finite difference) grid; these are explained in the settings section, see <u>3D Gridded Data</u>

The following is a list of the differences for unstructured grids:

- Under Cells, there is no option for "Show Only Borders"
- For Lines, there is no option for "Show Only Grid Frame"
- For Slice, there is an option "Show Cell ID Labels"; this will insert a label of the Cell ID for each cell in the selected slice. This will be useful if you want to adjust the numerical values for single cells (or a group of cells) using the Edit option described below.
- For Slice and ThreeSlices, the slice position for cross-sectional slices is based on a virtual grid; the unstructured grid is divided into 100 equally spaced rows and columns. You can display cross-sections through the USG, as "rows" or "columns", at positions from 1 100. Row 1 corresponds to the Y minimum in your model domain, whereas Row 100 corresponds to the Y maximum in your model domain. Column 1 corresponds to the X minimum in your model domain, whereas Column 100 corresponds to the X maximum in your model domain. The layer convention follows the MODFLOW notation, where Layer 1 is at the top.
- For Colormap, the positions are similar as to what you have for Slice described above. The option to display colormap along an arbitrary Cross-section line is currently not supported. For Colormap, there is an additional Slice Type, "Horizontal", which allows for rendering on a flat horizontal plane. In this case, you define the vertical position (shift) of this Horizontal plane, on a location from 1 - 100. Vertical Shift of 1 corresponds to the Z minimum in your model domain, whereas a shift of 100 corresponds to the Z maximum in your model domain. Only active cells in the model domain will be drawn.
- For Isolines (contour lines), the settings for selecting the plane for drawing the isolines are similar to described for Colormap above.

Export Properties

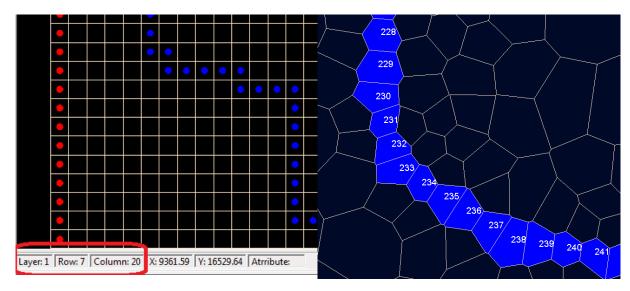
Any of the model properties can be exported to shapefile for further post-processing; see <u>Export</u> for more details.

11.3 Define Boundary Conditions

With an unstructured grid, boundary conditions are still defined at the cell-center, as with structured (finite difference) versions of MODFLOW. One of the biggest advantages of unstructured grids is that the cell sizes can be much smaller around these boundary conditions, providing for a higher level of accuracy and better representation. Furthermore, for Voronoi grids, the cell centroids can be made to align exactly with features of interest

such as stream channel centerlines and wells (please refer to the <u>Define Unstructured</u> <u>Voronoi Grid</u> section).

The other major differences lie in the way boundary condition cells are identified. With Structured MODFLOW (-2005, etc.), boundary condition cells are identified by row, column, layer, in their respective packages (.RIV, .WEL, .GHB, etc.). With unstructured grids, cells are identified by a CellID; after that, the parameters remain the same as what you see for structured MODFLOW.



MODFLOW-2005 grids, with cell numbering

MODFLOW-USG grid with CellID numbering

The CellD label for boundary condition cells can be turned on as described below.

Assign

The Assign button allows you to assign new boundary conditions. You have options to assign by Polyline or Polygon, by Using Data Object or by Cells. These options are described further below.

- **Polygon or Polyline**: Use this option to digitize one or more shapes and assign Boundary Condition attributes to the respective shapes. Use the left mouse button to start drawing and add attributes at the desired locations. Once you have finished digitizing, right click with the mouse to close the shape and select Finish button.
- Entire Layer (*Recharge and Evapotranspiration only*): Use this option when you want to assign a boundary condition to all cells in the layer.
- Using Data Object: Use this option when you have a polyline or polygon data object already imported into the projects, and you would like to use this shape to define the geometry.
- **Cells**: Use this option when you want to select individual cells to assign a boundary condition.

chedule Transien	it - 📪 🖷 🙀	Deer Cree	k-Zone	0 🔒 🏠 Calculatio	n 🗸	τ 💻 🔳 📰			
	erval to see the attributes of	Cell	V	River Stage (ft) ▼	Riverbed Bottom (ft)	Conductance (ft ² /day) T	Conc001 ₽	Active 5	7
the cells at that time.		▶ 103		583.3614401	580.3614401	257.7560257	0		
OK		103		583.4185774	580.4185774	257.7560257	0		
		103	3 5	583.5297087	580.5297087	257.756025	0	N	
Start Time	End Time	725	5	583.3450789	580.3450789	128.8780121	0	V	
0	1836.25	103	5 5	583.8240329	580.8240329	257,7560257	0		
		103	6 5	583.9183792	580.9183792	257.7560258	0		
		103	7 5	583.9605505	580.9605505	245.4815446	0		
		103	4 5	583.680859	580.680859	257.756025	0		
		104	2 5	584.0235437	581.0235437	234.0240815	0	N N N N	
		104	1 5	584.0114083	581.0114083	234.0240808	0		
		104	0 5	583.9162611	580.9162611	234.0240808	0		
		104	3 5	583.9905175	580.9905175	234.0240816	0		
		104	4 5	584.2065329	581.2065329	247.9082572	0		
		103	9 5	583.7842802	580.7842802	234.0240815	0		
		103	8 5	583.9871388	580.9871388	234.0240815	0	\checkmark	
		104	5 F	584 2925242	581 29253/3	261 8802759	n		

The Edit Boundary Condition attributes window will appear as shown below:

Enter the attributes using the various methods; click Finish when you are done. This dialog allows you to copy and paste from Excel to make defining (or editing) the attributes easy.

For more details on the options for defining attributes, see <u>Define Boundary Conditions</u> (<u>Attributes</u>).

If your boundary condition is transient switch the schedule drop down to transient to enter your schedule.

You can copy and paste your time schedule from Excel into this dialog to make defining your boundary condition quicker and easier.

By default the Assign to appropriate layer is selected. This means if you enter values for the attributes of a boundary condition (for example the Starting Head) which would place it into another layer - this will occur automatically once you save your boundary condition.

Edit

When you select the Edit... button you must select a cell containing the boundary condition you wish to edit.

Then the following dialog will appear (similar to defining the boundary condition):

hedule Transient	- 📪 🐺 🛛	Deer Creek-Zor	ne0 🎄 Calculation	\sqrt{x}			
elect a schedule interval	to see the attributes of	Cell 🛛	River Stage (ft) ₽	Conductance (ft^2/day) ₽	Conc001 ₽	Active V	
ne cells at that time.		1031	583.3614401	580.3614401	257.7560257	0	
OK		1032	583.4185774	580.4185774	257.7560257	0	
		1033	583.5297087	580.5297087	257.756025	0	\checkmark
Start Time	End Time	725	583.3450789	580.3450789	128.8780121	0	\checkmark
0	1836.25	1035	583.8240329	580.8240329	257.7560257	0	
		1036	583.9183792	580.9183792	257.7560258	0	\checkmark
		1037	583.9605505	580.9605505	245.4815446	0	
		1034	583.680859	580.680859	257.756025	0	
		1042	584.0235437	581.0235437	234.0240815	0	y y y
		1041	584.0114083	581.0114083	234.0240808	0	
		1040	583.9162611	580.9162611	234.0240808	0	
	-	1043	583.9905175	580.9905175	234.0240816	0	\checkmark
	1	1044	584.2065329	581.2065329	247.9082572	0	
		1039	583.7842802	580.7842802	234.0240815	0	
		1038	583.9871388	580.9871388	234.0240815	0	
		10/15	584 2925343	591 20252/2	261 8802759	Λ	

The attributes for each cell containing the boundary condition are displayed and can be edited. The cell you selected will be highlighted in the dialog. If you select other rows in the dialog - the corresponding cell will be highlighted in the viewer.

By default the "Assign to appropriate layer" option is selected. This means if you adjust the attributes of a boundary condition (for example the Stage) which would place it into another layer - this will occur automatically once you save your edits.

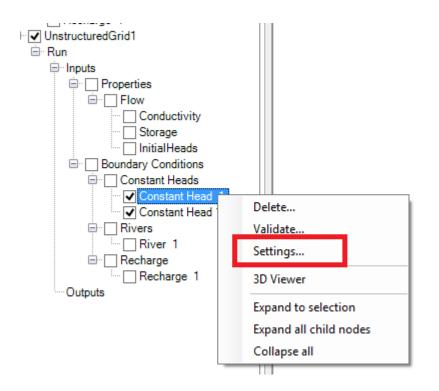
Script

If preferred you can make your boundary condition edits by using the Scrip option. On this tab you will find the script for any edits you make on the Edit cells tab allowing you to learn the script language. You can re-use the script to "replay" your edits to your boundary conditions.

Display Settings

The display settings can be launched by right-clicking on the desired object in the model tree, and selecting Settings...

Boundary condition cells can be shown:



The Settings window will load.

Boundary Condition cells can be drawn as Points (vertices) or as Cells

When selecting the Cells option, you will see the option "Show Cell ID labels"; turning this on will draw the Cell ID on top of the selected boundary condition cell type. This is useful if you wish to make edits to specific boundary condition attributes, as explained in the Edit section above.

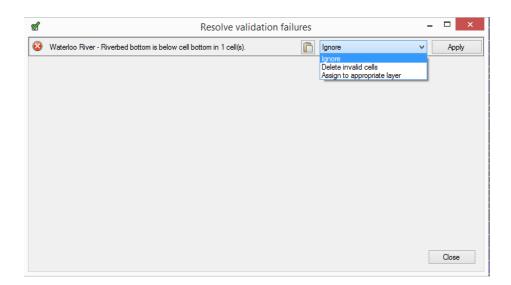
Delete

To delete a specific boundary condition cell group, right-click on this node in the tree, and select Delete.

Validation

To verify there are no warning or errors associated with a boundary condition, right-click one a specific boundary condition in the Model Explorer tree and select **Validate...** and if there are any errors or warnings, you will be provided with options to resolve the issue(s), as shown in the dialog below. This is available for Constant Head, River, General Head, and Drain boundary conditions. It will check to see if the attributes of the boundary condition will place it below the bottom of the cell you assigned it to. Then it will give you options to correct this. If you choose to Ignore the errors you may encounter errors when trying to translate and run your model.

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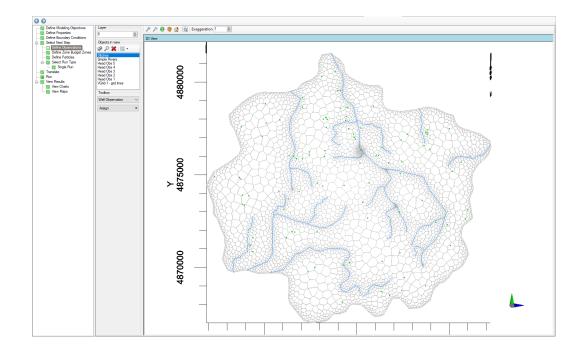


11.4 Define Observations

At the Define Observations step, you can define and edit observation data that can be used to compare your model to historical/expected values for various model outputs and evaluate your model results. The following types of observations can be added to a numerical model:

- Well Observations: heads or concentrations
- Zone Budget Obs: net volumetric flow exchange of groundwater
 - o in/out of a specified zone,
 - o between a specified zone and another zone, or
 - o between a specified zone and specified boundary condition type

Following a successful model run, assigned observations can be <u>compared</u> to simulated values to facilitate model evaluations including history matching/calibration.



Toolbar

Observations can be defined at the Define Observation step by selecting the type of observation to be defined under the toolbox and selecting the assign option:

• Under the Toolbox, use the combo box to select from the various Observation types:



• Then use the Assign button to assign the appropriate object type (described below) defining the observation location.

Well Observations

Well observations include groundwater data collected from wells and piezometers and consist of four components:

- Location: x- and y-coordinates of the sampling point
- **Elevation**: the elevation at which the observation occurred. For monitoring wells, this is typically the midpoint elevation of the screen. For pieozometers, this is typically the elevation of the open-ended bottom of the piezometer.
- **Time**: the time as an absolute date/time or more commonly as elapsed time relative to the model start date
- Value: the value of the observation:

- Head: the hydraulic head measured in the well or piezometer as top of casing elevation minus depth to water
- Concentration: solute concentration of the specified species (note that an extra field must be present to define the species)

Prerequisites

To define well observations, you must first have a well data object in the Data Explorer with observation data. You can either <u>import</u> the well observation data or create a new well data object and then add/edit the observation data. The "raw" observation well data can be viewed/edited in the <u>Well Data</u> section.

All other boundary conditions can be fully defined at the Define Observations step; however, you may find that using an imported <u>Time Schedule</u> object in the Data Explorer makes the process significantly more efficient.

Assigning the Well Observations

Once you have imported or created a <u>Well observation</u> data object with heads or concentrations, navigate to the Define Observations step in the numerical model workflow. Below the toolbox, select Well Observation and select Assign > using data object. The Create/Add Well Observations dialog will appear:

😂 Create/Add Well Observations			\times
Select a Well Observation object from the Data Tree:			
Assign observations to an existing well group			
Head Obs 1			~
O Assign observations to a new well group			
	OK	Can	cel

The Create/Add Well Observations dialog contains two controls:

- The assign button (): allows you to specify a well data object with observations in the Data Explorer
- The radio button allows you to specify which observation group the well observation object will be added to in the model tree.

The observation wells should then appear a new node on the numerical model tree on the Model Explorer and any observation well points located in the active layer, row, or column will be also be displayed in the appropriate view(s).

Please Note: If you add Observations that are defined in Absolute times and if some or all of the observation times occur before the model start date defined in the modeling objectives, then you will receive a warning message during creation. These head/concentration observations cannot be included in the numerical model and will be filtered out.

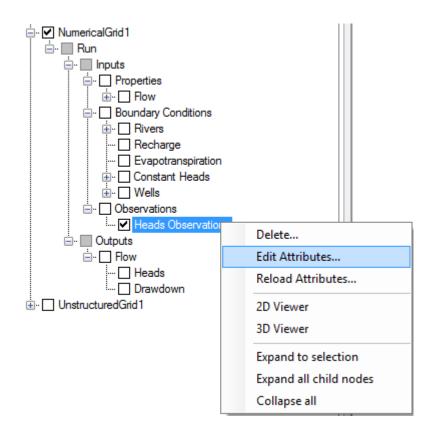
Specifying a Well Observation Group

You will be prompted with a choice to append the observations to an existing well group or create a new well group. Well groups can be used to group observation data into logical sets of data based on a meaningful criteria that may facilitate model calibration, analysis, or evaluation. For example you may wish to group observations by watershed, hydrostratigraphic unit/zone, landuse, or property type.

Viewing and Editing Well Observations in CSV Format

Once defined, head or concentration observation data can be viewed/modified in a CSV format:

- Right-click on the Head (or Concentration) Observations node from the Model explorer
- Select "Edit Attributes..." as shown below.



The data contained inside the Observations data object will be displayed in a .CSV file; this should appear in either Notepad or Excel depending on your system configuration; an example is below:

Ŕ	AutoSave 💽 Of		1 🔒 🗘	≂	16415557-d6	670-4dd5-89	a5-7aa300d9	960a8.csv 🝷		Search
F	File <u>Home</u> Ins	ert Draw	/ Page La	ayout Fo	ormulas [Data Re	view Viev	v Develo	per Help	Team
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$										
Undo Clipboard 🖾 Font 🖾 Alignment 🖾 No										L2
A1 \checkmark : $\times \checkmark f_x$ Well Name										
	А	В	с	D	E	F	G	н	1	J
1	Well Name	X(m)	Y(m)	Obs. ID	Obs. Elev.	Layer	Obs. Time	Head(m)	Target Resid	ual
2	obore_1/obore_1	131.25	65	Observati	30	1	3.516991	52.6047	1	
3	obore_1/obore_1	131.25	65	Observati	30	1	7.737998	51.54321	1	
4	obore_1/obore_1	131.25	65	Observati	30	1	12.80199	50.67741	1	
5	obore_1/obore_1	131.25	65	Observati	30	1	18.88	49.96522	1	
6	obore_1/obore_1	131.25	65	Observati	30	1	26.173	49.39998	1	
7	obore_1/obore_1	131.25	65	Observati	30	1	34.925	48.97589	1	
8	obore_1/obore_1	131.25	65	Observati	30	1	45.42699	48.67857	1	
9	obore_1/obore_1	131.25	65	Observati	30	1	58.02939	48.48562	1	
10	obore_1/obore_1	131.25	65	Observati	30	1	73.15238	48.37075	1	
11	obore_1/obore_1	131.25	65	Observati	30	1	91.3	48.30856	1	
12	obore_1/obore_1	131.25	65	Observati	30	1	94.81712	48.84876	1	
13	obore_1/obore_1	131.25	65	Observati	30	1	99.03767	49.3166	1	
14	obore_1/obore_1	131.25	65	Observati	30	1	104.1023	49.72452	1	
15	obore_1/obore_1	131.25	65	Observati	30	1	110.1799	50.06768	1	
16	obore_1/obore_1	131.25	65	Observati	30	1	117.4731	50.34068	1	
17	obore_1/obore_1	131.25	65	Observati	30	1	126.2248	50.54399	1	
18	obore_1/obore_1	131.25	65	Observati	30	1	136.7269	50.6845	1	
19	obore_1/obore_1	131.25	65	Observati	30	1	149.3294	50.77394	1	
20	obore_1/obore_1	131.25	65	Observati	30	1	164.4524	50.82594	1	
21	obore_1/obore_1	131.25	65	Observati	30	1	182.6	50.85334	1	
22	obore_1/obore_1	131.25	65	Observati	30	1	186.1171	51.53153	1	
23	obore_1/obore_1	131.25	65	Observati	30	1	190.3377	52.10756	1	
24	obore_1/obore_1	131.25	65	Observati	30	1	195.4023	52.60427	1	
25	obore_1/obore_1	131.25	65	Observati	30	1	201.4799	53.01608	1	

You can use this interface for numerous types of edits/additions:

- Adding a new observation point at a defined XY location
- Change existing data
- Add a new observation time to an existing observation point.

Please Note: the Layer number for the observation point is calculated based on the Obs. Elev; changing the layer number will not change the vertical location of the observation point.

When you are finished with the edits in the .CSV file, you need to save and close this file. Then re-import back the changes into Visual MODFLOW Flex using the steps below:

- Right-click on the Head (or Concentration) Observations node from the Model explorer
- Select "Reload Attributes..."

The modified data will now appear and will be utilized for any charts the next time you translate and run the model.

Defining Zone Observations

Visual MODFLOW Flex allows you to define observations of net volumetric flows using ZoneBudget zones.

Assign ZoneBudget Observations

To define a boundary condition observation data set:

- At the Define Observations step, select the Zone Budget Obs option in the toolbox
- Click Assign > Using data object...
- The Gage Editor window will be displayed allowing you to define the observations

🂐 Gage I	Editor							×
ditor So	nipt							
iage Type	Volumetric Flow + ft^3	/d 🛺 🙀 🙀				Gage station name		
		\overline{x}						
Time		Value	V	Target Residual	V			
(31	145.1102643		5		Selected zone (From):		
•	60	112.8110465		5		Zone 1	\sim	
	91	141.8077018		5				
	121	111.6546235		5		Select zone (To)		
	152	55.67374097		5		2 (B 1 1 1)		
	182	69.36806236		5		Zone / Boundary condition		1
	213	102.1205018		5			~	Т
	244	148.2311585		5		Zone 2		
ſ	274	118.2628886		5		Zone 3		
	305	52.55330493		5		Constant Head	NA	1
	335	115.9618202		5		River	NA	J.
*								
_								
Load	schedule object			 Load 			OK Can	cel

Observation Schedule

The left side of the Gage Editor dialog includes the following controls for all supported types of distributed (non-point) observations (zone budget zones):

• **Gage Type**: allows you to select the type of observation to be measured and associated project <u>units</u>. Currently, distributed non-point gages/observation types are

limited to volumetric observations. Note that well observations are handled separately using well objects (see above).

- **Toolbars:** the gage toolbars include the following buttons:
 - o Add interval: adds an observation time at the end of the table
 - o 🖽 Insert interval after selection: adds an observation time after the selected row
 - Delete selected row(s): deletes selected row(s) from the table
 - o Section 2 Clear sort: clears the sort order (if any) on fields in the observation table
 - $\circ \sqrt{x}$ Expression builder: opens the Expression builder
 - o III Assign to column: evaluates the Expression for all cells in the current column
 - Assign to current cell: evaluates the Expression for all selected cells in the current column (press and hold SHIFT or CTRL buttons with left mouse clicks to select multiple cells)
- Table: the table in the left hand side of Gage Editor includes three fields:
 - o Time: elapsed time relative to the model start date
 - Value: the value of the observation. Note that positive flow values for volumetric observations follow the standard MODFLOW convention that positive values indicate flow <u>into</u> the groundwater flow system
 - *Target Residual*: the target difference between observed values and simulated results (based on project goals, stakeholder input).
- Load Schedule Object: Selecting this option will allow you to load the data from a time schedule object in the Data Explorer and map fields from the schedule object (using the dropdown selectors) to the value and target residual fields.

Gage schedule field mapping		_	- [×
Zone Budget-Gage 3					
Gage field	Project unit	Schedule field			
VolumetricFlow	ft^3/d	Value			
VolumetricFlow (Residual)	ft^3/d	Target Residual			\sim
		None			
		Value			
		Target Residual			
			OK	Car	ncel .:

Zone Budget Observation Spatial Representation

The right side of the Gage Editor includes the spatial definition of the observation:

- Selected Zone (From): The "from" zone selection allows you to specify the zone where groundwater flows are to be observed.
- Selected Zone (To): The "to" zone selection (shown in red) is optional and allows you to specify a different ZoneBudget zone or a boundary condition type present in the model. If not selected, then the net groundwater flows to all adjacent zone budget zones will be observed.

Script

The Script tab allows you to quickly add or modify data based on a script. If you are interested in using the script, try to define a simple gage to observe the structure and add complexity. An example is shown below:

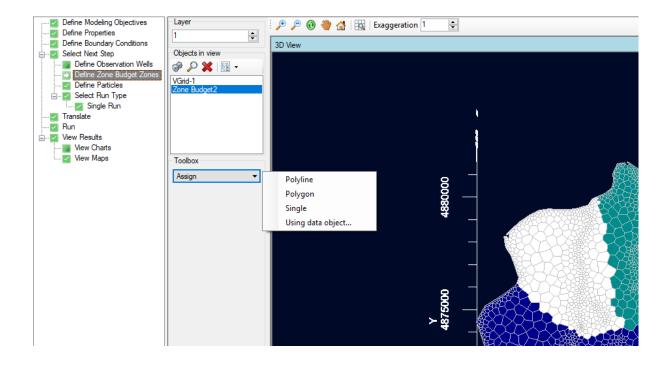
۹ 🔍	age Editor		_		×
Editor	Script				
1 2 3 4 5 6	StationScope = Riv ZBPlugin = fbd700ad-4a <u>11-4f03-83ff-5defd0</u> Selection = ZoneBC1 {				^
7 8 9	ZoneId = 1 BCType = RIV }	- Observation Scope			
10 11 12 13	X = 486574.007 Y = 4876771.843 Z = 320.498644808286 StationData =	– Location			
14 15 16	GageType = VolumetricFlow ObservationSet = 31 148.4519084 10	 Observation Type 			
17 18 19	60 148.4491265 10 91 161.1939558 10 121 146.0752151 10				
19 20 21 22 23 24 25 26	121 146.072151 10 152 155.0165833 10 182 146.3191499 10 213 149.6536931 10 244 143.6346395 10 274 144.6857469 10 305 144.0838687 10 335 159.655898 10	- Observation Data			
27	366 154.4116067 10				~
	Load schedule object	✓ Load QK		<u>C</u> ance	el

- The header defines the type of observation and (other than the name, which should be wrapped in "quotes") should not be edited.
- The **Observation Scope** section defines which objects are associated with the observation gage.
- The **Location** section defines where the observation will be rendered in views when displaying residuals
- The **Observation Type** defines which observation data are used. You can specify more than one Observation Type block
- The **Observation Data** includes the set of times, observations, and target residuals for the time above.

Similar to a macro builder, any edits you make on the Edit tab will be reflected at the Script tab. In this way you can experiment with the Gage Editor and learn to build your own scripts.

11.5 Define Zone Budget Zones - USG

ZoneBudget-USG and ZoneBudget-6 are USGS programs for computing subregional water budgets for MODFLOW ground-water flow models using unstructured grids. At the Define Zone Budget Zones step, you can create or assign zone budget zones by digitizing new zones using Assign Polyline, Polygon, or Point (Single Cell), or by using 2D/3D point, polyline, or polygon shape objects from the Data tree using the same methods as in the Finite Difference workflow.



Follow the steps below to create new zone budget zones:

Assign

Polyline

• Use the left mouse button to start digitizing a polyline over the desired cells. Once you have finished digitizing, click on the Finish button from the toolbox, or right click with the mouse and select "Define Attributes". The following window will appear

Create new zone budget zone
Assign to single zone
Select zone:
Zone 1 V New
Create new zones from attribute
No attributes 🗸 🗸
Use integer field values
Assign to layer
Assign to all layers
<pre> Layer 1 Layer 2 Layer 3 Layer 4 Layer 5 Layer 6 </pre>
OK Cancel Help

• Click the New button to assign the selected cells to a New zone; otherwise, you can select to assign cells to an existing zone by selecting the zone from the dropdown list at the top. The selected cells can be assigned to the current layer or multiple layers using the check boxes at the bottom of the window. Once you are finished, click OK.

Polygon

• Digitize one or more polygons, and repeat the steps as described above for Polylines.

Single

• Left-click on one or more cells and a point will appear. Once finished, right-click and select "Define Attributes", and follow the steps as described above for Polylines.

Using Data Object....

• The following window will appear.

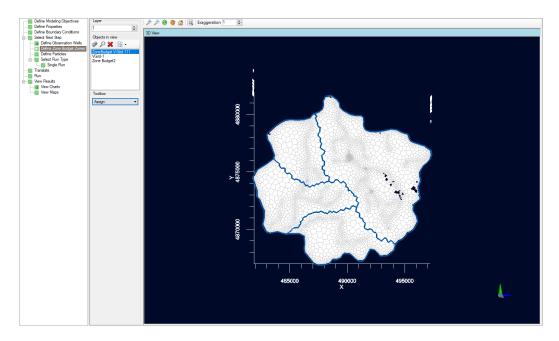
Select geometry object	x
Select a points, polyline or polygon data object	
<u>O</u> K <u>C</u> an	cel

- Choose the desired point, polyline, or polygon data object from the tree.
- Click on the button (under Select Data Object)
- A second window will appear:

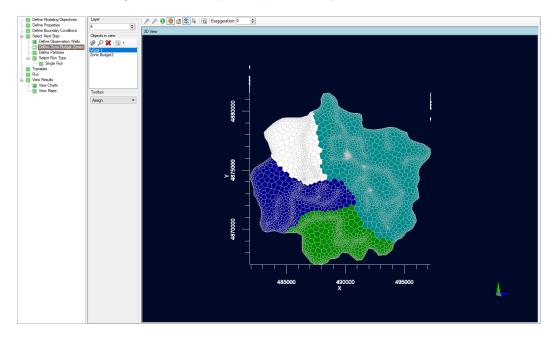
Create new zone budget zone
O Assign to single zone
Select zone:
Zone 1 Vew
 Create new zones from attribute
Zone ~
Use integer field values
Assign to layer Assign to all layers Layer 1 Layer 2 Layer 3 Layer 4 Layer 5
Layer 6
OK Cancel Help

- Select which zone you want the features to apply to. You have the option to assign the zones to:
 - $_{\rm O}\,$ An existing zone
 - A new single zone
 - o Create zones for individual features
 - o Create zones based on feature attributes
- Select the desired model layers where the zone should be applied

A simple example is shown below for a polygon data object (shown in blue).



After the zones are generated, they will appear in layer view.

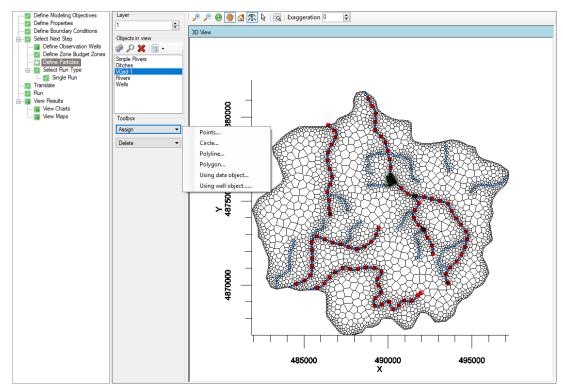


When the selected shape contains multiple polyline or polygon features, then a new zone will be created for each feature.

11.6 Define Particles

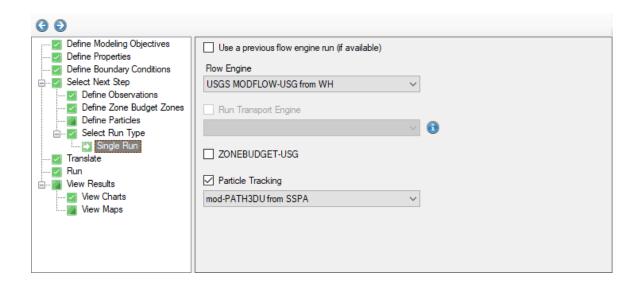
910

Particles are defined using the same methods as in the Finite Difference workflow. These methods are described in the section describing how to <u>Define Particles</u> in the Finite Difference workflow.



11.7 Select Engines

The Single Run workflow step is used to select the Flow Engine and associated utilities (e.g. ZoneBudget and mod-PATH3DU) you wish to include in the model run. Visual MODFLOW Flex requires you to select a flow engine for a particular run. Running a particle track engine and/or ZoneBudget is typically optional.



When you are finished selecting which engine(s) to run, click 😒 (Next Step) button to proceed.

Engines Supported in the Finite Difference Numerical Workflow

The table below lists all supported engines and utilities supported in Visual MODFLOW Flex for unstructured grids.

Flow	Transport	Utilities
MODFLOW-USG	• N/A	 ZONEBUDGET- USG and MOD-PATH3DU
MODFLOW-6	MODFLOW-6	• ZONEBUDGET-6

Engines supported in the Numerical Workflow

 MODFLOW-6 includes a number of significant differences when compared to other engines. If you are not familiar with MODFLOW-6 and how it has been implemented in Visual MODFLOW Flex, at a minimum, please read the the <u>Introduction to MODFLOW-6</u> as well as the discussions about translating MODFLOW-6 groundwater flow (<u>GWF</u>) and (<u>GWT</u>) models. When you are finished, click 🕏 (Next Step) button to proceed.

Using a Previous Flow Engine Run

When running a transport simulation or a utility, in order to save some time, you may wish to reuse the results of a previous flow engine run, particularly if you need to rerun the configuration repeatedly. Provided you have run the flow engine at least once, you can select the "Use a previous flow engine run (if available)" option. If this option is selected and you proceed to the <u>Translation</u> step, the flow engine settings will be hidden, since the previous flow engine settings will be reused.

11.8 Translation Settings

The translate step allows you to translate the model into the input files that the applicable engine(s) will run. There are also settings for each engine that allow you to make adjustments to how the model is run (e.g. solver settings, alternative initial heads, output control, and individual package settings).

The translation step consists of two vertical panels. The left panel includes a tree structure that lists the engine(s) selected at the <u>Select Engines</u> step and associated settings for each applicable engine. The panel on the right displays the settings (and controls) for the selected node on the translation tree. Each sub-topic in this section of the documentation describes the available settings for each node on the translation tree.

Define Properties Define Properties Define Properties Define Cherral	Define Modeling Objectives		00																
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² Define Observations ² Selet Run Type ² Selet Run Type ² Selet Run Type ² Selet Run Type ² Output Folder ² Output Folder ² Output Folder ² View Results ² Output Control ² Output Control ² Output Control ² Output Control ² View Maps ² Moreneutrations ² Output Control ² Advanced Settings ³ View Maps ⁴ Maximed Settings ⁴ Maximed Settings ⁴ View Maps ⁴ Maximed Settings ⁴ Output Control ⁴ Advanced Settings ⁴ Advanced Settings ⁴ Output Control ⁴ Advanced Settings ⁴ Output Control ⁴ Output Control ⁴ Advanced Settings ⁴ Output Folder ⁴ Output Folder		Settings	Translation Log	nam	TDIS	IMS	DISV	IC	OC	NPF	CHD	CHD(2)	RIV	RIV(2)	RIV(3)	RIV(4)	STO	GHB	• •
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Output Folder			Output Control																
			Advanced Setting	s															
					O	tout Fol	der												

Tools

The following tools and buttons are available at the translation step:

- Translate Translate: initiates model translation
- Open: opens a file dialog in the folder path of the current run so that you can select and open a model input file.
- Tabs: toggles the layout of the translated tabs tabs can be displayed along a single line with scrolling arrows (default) or along multiple lines.
- S Previous/Next Error: jumps to the previous/next error or warning in the translation log.

Upon translation of your model, Visual MODFLOW Flex will open a new tab that displays the translation log, and convert input data for the current run in the workflow in the model explorer to that input data files required for the selected numeric engines (see <u>Appendix A</u> for details) - one tab is added to for each model package in the run. You can click any of these packages to view the contents of the corresponding input file. You can also edit these and save your changes by right-clicking in the package window and selecting save or by

typing <u>(CTRL)</u>. Note that your changes will be overwritten if you re-translate your model and the package advanced <u>setting</u> for translation is set to"Yes".

General Settings

At the General Settings page you can see the following information:

- Output Directory: the folder path where the translated engine files are stored.
- Model Start Date: the start date will be the same as that which you specified in the Define Modeling Objectives step.

Engine/Package Translation Settings

This chapter covers the following topics:

- MODFLOW-USG Translation Settings:
 - o <u>Solvers</u>
 - o Initial Heads
 - o Output Control
 - o Advanced Settings
- MODFLOW-6 Translation Settings*:
 - o <u>General</u>
 - MODFLOW-6 Settings
 - o <u>Solver Settings</u>
 - o Initial Heads
 - o Output Control

- o Advanced Settings
- MODFLOW-6 Transport Translation Settings*:
 - o General Settings
 - o Solver Settings
 - o Initial Concentrations
 - o Output Control
 - o Advanced Settings
- * Note: MODFLOW-6 includes a number of significant differences when compared to other engines. If you are not familiar with MODFLOW-6 and how it has been implemented in Visual MODFLOW Flex, at a minimum, please read <u>Introduction to</u> <u>MODFLOW-6</u> and the settings listed above.
- MOD-PATH3DU Translation Settings

11.8.1 MODFLOW-USG

The adjustable settings available for the MODFLOW-USG engine are described below.

MODFLOW-USG Settings

Property Package: available options are:

- Layer Property Flow (LPF) (default) or
- Block-Centered Flow (BCF)

Run Type: Steady-State or Transient

If the Steady-State Flow option is selected, Visual MODFLOW Flex will prepare the data set for a steady-state flow simulation, and will automatically use the data from the first time period (only) of each boundary condition and pumping well defined in Visual MODFLOW Flex to run the model to achieve flow equilibrium (i.e. a time-independent solution since all inputs are constant).

Please Note: if running a steady-state model, at least one boundary condition with a head of known elevation must be specified (e.g. constant head, river stage, drain bottom, general head elevation).

If the Transient Flow option is selected, Visual MODFLOW Flex will prepare the data set for a transient flow simulation. During this process, Visual MODFLOW Flex will automatically merge all of the different time period data defined for each pumping well and boundary condition into the stress period format required by the applicable engine. This creates a time-dependent flow solution, as the model is being run with different inputs at different times.

Steady-State Simulation Time: specified time for the mass balance terms in a steady-state run.

Settings Translation Log		
 General Settings MODFLOW-USG Settings Solvers Initial Heads Output Control Advanced Settings MOD-PATH3DU Settings 	General Property Package Run Type Steady-State Simulation Time	LPF Steady-State 7300
	Run Type Simulation Type: Steady-State or Transient	

Stress Periods and Time Steps

The Time Steps option is only available when you are running a transient model (i.e. when Transient Flow run type is selected). For transient flow simulations, Visual MODFLOW Flex will automatically merge all of the different time periods defined for all of the different pumping wells and boundary conditions into the uniform stress period format required by MODFLOW. A stress period is defined as a time period in which all the stresses (boundary conditions, pumping rates, etc.) on the system are constant. Unfortunately, the data collected for each modeling site is rarely synchronized in terms of stress periods, so Visual MODFLOW Flex merges the time schedules for all pumping wells and boundary conditions to determine the length of each stress period for a transient simulation. As a result, the user cannot directly modify the number of stress periods or the length of each stress period.

The Time step options window (as shown in the following figure) is used to define the number of Time steps in each stress period and the time step Multiplier is used to increment each time step size.

Settings Translation Log									
🗐 General	✓ General								
Settings	Property Package	Property Package			LPF				
. MODFLOW-USG	Run Type	Run Type			Transient				
Settings	Steady-State Simu	Steady-State Simulation Time			7300				
···· Solvers									
Initial Heads									
Output Control									
Advanced Settings									
MOD-PATH3DU									
: Settings									
	Property Package								
	LPF and BCF packages can be used for MODFLOW USG.								
	Time Steps Value								
	Stress Period	Start	End	Time Steps	Multiplier	Steady-State			
	1	0	3650	20	1.2				

The Stress Period column indicates the stress period number while the Start and End columns indicate the start time and end time, respectively, for each stress period.

Each stress period is divided into a user-defined number of Time steps whereby the model will calculate the head solution at each time step. The default value for Time steps is 10.

The time step Multiplier is the factor used to increment the time step size within each stress period (i.e. it is the ratio of the value of each time step to that of the preceding time step). The default value is 1.2. A time step Multiplier value greater than 1 will produce smaller time steps at the beginning of a stress period resulting in a better representation of the changes of the transient flow field. Thus increasing the number of time steps in a simulation may result in smoother head or drawdown versus time curves.

The steady-state column indicates if the stress period is transient or steady-state. Steadystate and transient stress periods can occur in any order. Commonly the first stress period may be run as steady state, to produce a solution that is used as the initial condition for subsequent transient stress periods.

Accommodating Boundary Conditions with Varying End Times

Visual MODFLOW Flex allows you to define boundary conditions with varying end times; the number of stress periods for the model will be calculated from the end time of the longest boundary condition. If there is a stress period where there are no data defined for a boundary condition, then you will see an entry of "0" in the appropriate package, for that stress period; this denotes that zero cells are defined for that stress period. In the case of pumping wells, you will see a rate of 0 for the well cells.

The settings for some of the other packages can be adjusted as per the sections below.

For more details, please refer to the MODFLOW-USG version 1.4.00 manual, by Panday et al. (2013), which is available from the USGS website: <u>http://water.usgs.gov/ogw/mfusg/</u>

Layer Types

By default, the layer type is set as 4, for both the .BCF and .LPF packages. The layer types can be adjusted at the top of each respective package.

Time Steps

The number of time steps for each stress period is defined at the end of the .DISU package; simply open this tab, change the desired value, save the package, then proceed with the run.

Output Control

The OC package for MODFLOW-USG uses text keywords, making it simpler to understand the file format. By default, heads and drawdown will be saved for every time step, up to 10 time steps per stress period. If you change the number of time steps, then you may need to update the Output control, to save heads/drawdowns at the desired time steps.

SMS Package

The parameters for the .SMS package are described in the MODFLOW-USG manual, and in the "MODFLOW-USG Version 1.4: Description of Model Input and Output". In addition to the options described in the manual, you can also choose to use the SAMG solver for the matrix solution method (i.e. LINMETH=3).

BAS Package and Discontinuous Layers

Visual MODFLOW Flex assumes that all layers have the same horizontal discretization. When there is a layer that pinches out, resulting in a cell thickness of zero, these cells will not be displayed in the 3D viewer. During the translation to MODFLOW-USG packages, the cells with zero thickness will be marked as inactive in the basic (.BAS) package and in the .DISU (UnStructured Grid) package, those zero thickness inactive cells have no vertical connections. Their upper and lower neighbors are directly connected together, effectively bypassing the inactive cells with zero-thickness.

11.8.1.1 Solvers

Solvers in MODFLOW-USG are handled through the Sparse Matrix Solver (SMS) package. The SMS package uses a combination of strategies including: preconditioning, acceleration, linear and non-linear methods, ordering, and term dropping to solve the simultaneous equations produced by the model as described below.

General Solution Method Parameters

The following parameters and settings are always incorporated in the SMS package.

Pre-defined input values (OPTIONS)

An optional keyword setting that activates solver options:

- *SIMPLE* indicates that default solver input values will be defined that work well for nearly linear models. This would be used for models that do not include nonlinear stress packages (e.g. UZF, SFR) and models that are either confined or consist of a single unconfined layer that is thick enough to contain the water table within a single layer.
- MODERATE indicates that default solver input values will be defined that work well for moderately nonlinear models. This would be used for models that include nonlinear stress packages and models that consist of one or more unconfined layers. The "MODERATE" option should be used when the "SIMPLE" option does not result in successful convergence.
- COMPLEX indicates that default solver input values will be defined that work well for highly nonlinear models. This would be used for models that include nonlinear stress packages and models that consist of one or more unconfined layers representing complex geology and sw/gw interaction. The "COMPLEX" option should be used when

the "MODERATE" option does not result in successful convergence.

• CUSTOM indicates that no keyword will be included and the full list of applicable settings will be translated into the SMS package.

Please Note: when using the SIMPLE, MODERATE, and COMPLEX options, only the following parameters are included in the SMS package: HCLOSE, HICLOSE, MXITER, ITER1, IPRSMS, NONMETH, LINMETH. The defaults are used for the remaining settings.

Head Change Criterion (HCLOSE)

The head change convergence criterion for nonlinear problems. HCLOSE can be any positive value; the default is 1.0E-5.

Head Change Criterion for Convergence (HICLOSE)

The head change convergence criterion for inner iterations. HICLOSE can be any positive value; the default is 1.0E-5.

Max. Outer Iteration (MXITER)

The maximum number of outer iterations. MXITER can be any positive integer value; the default value is 500.

Max. Inner Iteration (ITER1)

The maximum number of inner iterations for each linear solution. ITER1 can be any positive integer value; the default value is 1600.

Printing Convergence Info (IPRSMS)

Controls printing of convergence information from the solver in the Listing file.

- Don't display convergence information (0): excludes solver information from the listing file
- Display total iterations and summaries (1): includes the total number of inner/outer iterations and the nonlinear residual reduction summaries [default]
- Display all available information (2): includes the information above, plus matrix solver information

Nonlinear Solution method (NONLINMETH)

Controls the nonlinear solution method and under-relaxation schemes. The absolute value of NONLINMETH determines the underrelaxation scheme used, while the sign determines the iteration scheme:

• *O*: Picard iteration scheme is used without any under-relaxation schemes involved

- < 0: Picard iteration scheme is used with under-relaxation.
- > 0: Newton-Raphson iteration scheme is used with under-relaxation.
- 1 or -1 : Delta-Bar-Delta under-relaxation is used.
- 2 or -2 : Cooley under-relaxation scheme is used.

The default is 2 which corresponds to Newton-Raphson iteration with Cooley underrelaxation

Linear Solution Method (LINMETH)

The SMS package includes the option to use one of three solvers:

- Use Ibaraki chi-MD matrix solver (LINMETH=1): an asymmetric matrix solver called xMD (chi-MD) (Ibaraki, 2005),
- Use White-Hughes matrix solver (LINMETH=2): an unstructured preconditioned conjugate gradient (PCGU) solver developed by White and Hughes (2011) for symmetric equations, and
- Use SAMG matrix solver (LINMETH=3): the advanced/proprietary SAMG solver developed at the <u>Frauenhofer Institute</u>.

Non-linear Solver Parameters

The delta-bar-delta algorithm is a pre-conditioning method that is based on neural networks that uses results from previous iterations to inform the direction and magnitude of cell-by-cell under-relaxation. The Cooley scheme is a less-memory intensive alternative to the delta-bar-delta scheme.

The following parameters complement the gradient-based solutions and define how much and what components of the previous results are used to inform the overall search gradient relative to the search gradient determined by the linear solution method alone:

Reduction Factor for Learning Rate of Delta-Bar-Delta algorithm (THETA)

If the change in the head is of opposite sign to that of the previous iteration, the underrelaxation term is reduced by a factor of THETA. THETA can be any value from 0 to 1 and usually ranges from 0.3 to 0.9. The default value is 1.0 but a value of 0.7 works well for most problems.

Learning Rate Increment (AKAPPA)

The increment for the learning rate (under-relaxation term) of the delta-bar-delta algorithm. If the change in the head is of the same sign to that of the previous iteration, the under-relaxation term is increased by an increment of AKAPPA. AKAPPA can be any value from 0 to 1 and usually ranges from 0.03 to 0.3. The default is value is 0 but a value of 0.1 works well for most problems.

Memory term factor (GAMMA)

The history or memory term factor of the delta-bar-delta algorithm. The memory term is maintained as an exponential average of past changes. Retaining some past history can overcome granular behavior in the calculated function surface and therefore helps to overcome cyclic patterns of non-convergence. When GAMMA is zero, only the most recent history (previous iteration value) is maintained. As GAMMA is increased, past history of iteration changes has greater influence on the memory term. GAMMA can be any value from 0 to less than 1 and usually ranges from 0.1 to 0.3. The default value is 0.1, but a value of 0.2 works well for most problems.

Fraction of past history added (AMOMENTUM)

The fraction of past history changes that is added as a momentum term to the step change for a nonlinear iteration. A large momentum term should only be used when small learning rates are expected. Small amounts of the momentum term help convergence. AMOMENTUM can be any value from 0 to 1 and usually ranges from 0.0001 to 0.1. The default value is 0, but a value of 0.001 works well for most problems.

Backtracking Iterations Allowed (NUMTRACK)

The maximum number of backtracking iterations allowed for residual reduction computations. If NUMTRACK = 0 then the backtracking iterations are omitted. NUMTRACK can be any non-negative integer and usually ranges from 2 to 20. The default is 0 and a value of 10 works well for most problems.

Residual Change Tolerance (BTOL)

The tolerance for residual change that is allowed for residual reduction computations. BTOL should not be less than one to avoid getting stuck in local minima. A large value serves to check for extreme residual increases, while a low value serves to control step size more severely. The value usually ranges from 1.0 to 106; a value of 104 works well for most problems but lower values like 1.1 may be required for harder problems.

Step Size Reduction (BREDUC)

The reduction in step size used for residual reduction computations. BREDUC can be any value from 0 to 1 and usually ranges from 0.1 to 0.3. The default value is 0.1 and a value of 0.2 works well for most problems.

Residual reduction limit when backtracking (RESLIM)

The limit to which the residual is reduced with backtracking. If the residual is smaller than RESLIM, then further backtracking is not performed. A value of 100 is suitable for large problems and residual reduction to smaller values may only slow down computations.

Parameters for the Ibaraki xMD Solver

The following parameters are used by the Ibaraki _xMD Solver:

Acceleration method flag (IACL)

The flag for choosing the acceleration method.

- Conjugate Gradient (0): select this option if the matrix is symmetric. [Default]
- ORTHOMIN (1)
- BiCGSTAB (2)

Ordering Scheme Flag (NORDER)

The flag for choosing the ordering scheme.

- Original ordering (0) [Default]
- Reverse Cuthill McKee ordering (1)
- Minimum degree ordering (2)

Fill Level for ILU Decomposition (LEVEL)

The level of fill for ILU decomposition. Higher levels of fill provide more robustness but also require more memory. For optimal performance, it is suggested that a large level of fill be applied (7 or 8) with use of drop tolerance. The default value is 3.

Number of Orthogonalizations (NORTH)

The number of orthogonalizations for the ORTHOMIN acceleration scheme. A number between 4 and 10 is appropriate. Small values require less storage but more iteration may be required. This number should equal 2 for the other acceleration methods.

Reduced System Index (IREDSYS)

The index for creating a reduced system of equations using the red-black ordering scheme:

- No reduced system of equations (0) [Default]
- Create reduced system using red-black ordering (1)

Residual Tolerance Criterion (RRCTOL)

A residual tolerance criterion for convergence. The root mean squared residual of the matrix solution is evaluated against this number to determine convergence. The solver assumes convergence if either HICLOSE (the absolute head tolerance value for the solver) or RRCTOL is achieved. Note that a value of zero ignores residual tolerance in favor of the absolute tolerance (HICLOSE) for closure of the matrix solver.

Drop Tolerance (IDROPTOL)

The flag to perform drop tolerance:

- 0 do not perform drop tolerance
- 1 perform drop tolerance [Default]

Drop Tolerance Value (EPSRN)

The drop tolerance value. A value of 10⁻³ works well for most problems.

Parameters for the Hughes-White PCGU Solver

The following parameters are used by the Hughes-White PCGU Solver:

Linear Acceleration Method (CLIN)

An option keyword that defines the linear acceleration method used by the PCGU solver.

- Preconditioned conjugate gradient method (CG) [Default]
- Preconditioned bi-conjugate gradient stabilized method (BCGS)

The preconditioned conjugate gradient method should be used for problems with a symmetric coefficient matrix. The preconditioned biconjugate gradient stabilized method should be used for problems with a non-symmetric coefficient matrix (for example, with problems using the Newton-Raphson linearization scheme).

Pre-Conditioner Flag (IPC)

A flag for choosing a matrix preconditioner:

- No preconditioning (0)
- Jacobi preconditioning (1)
- ILU(0) preconditioning (2)
- MILU(0) preconditioning (3) [Default]

Matrix Scaling Approach Flag (ISCL)

A flag for choosing the matrix scaling approach used:

- No matrix scaling applied (0) [Default]
- Symmetric matrix scaling (POLCG) (1): use the POLCG polynomial preconditioner scaling method by Hill (<u>1990</u>).
- Symmetric matrix scaling (L-squared norm) (2): use the I2 norm of each row of A (DR) and the I2 norm of each row of DRA.

If the ILU(0) or MILU(0) preconditioners are used (IPC = 2 or 3) and matrix reordering is selected(IORD > 0), then ISCL must be 1 or 2.

Matrix Reordering Approach Flag (IORD)

A flag for choosing the matrix reordering approach used:

- Original ordering (0) [Default]
- Reverse Cuthill McKee ordering (1)
- Minimum degree ordering (2)

If reordering is used, reverse Cuthill-McKee ordering has been found to be a more effective reordering approach for the test problems evaluated.

Flow Residual Tolerance for Convergence (RCLOSEPCGU)

A real value that defines the flow residual tolerance for convergence of the PCGU linear solver. This value represents the maximum allowable residual at any single node. Value is in units of length cubed per time, and must be consistent with MODFLOW-USG length and time units. Usually a value of 0.1 is sufficient for the flow-residual criteria when meters and seconds are the defined MODFLOW-USG length and time.

Relaxation Factor (RELAXPCGU)

A real value that defines the relaxation factor used by the MILU(0) preconditioner. RELAXPCGU is unitless and should be greater than or equal to 0.0 and less than or equal to 1.0. RELAXPCGU values of about 1.0 are commonly used, and experience suggests that convergence can be optimized in some cases with RELAXPCGU values of 0.97. A RELAXPCGU value of 0.0 will result in ILU(0) preconditioning.

RELAXPCGU is only specified if IPC=3. If RELAXPCGU is not specified and IPC=3, then a default value of 0.97 will be assigned to RELAXPCGU.

Update Solvers

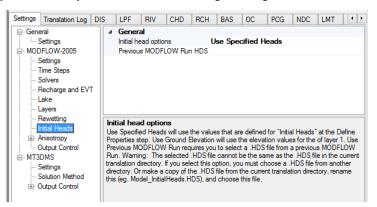
The update solver [Update Solver] button allows you to update/translate the solver package settings, since it is common to adjust only the solver settings when (re)-running a model. This allows you to quickly readjust the values more efficiently than translating the whole model.

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11.8.1.2 Initial Heads

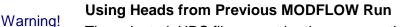
In Visual MODFLOW Flex, the Initial Heads are defined at the stage of Defining the Properties. For more details, please see the section on setting <u>Initial Heads</u> in the Define Properties workflow step.

When translating your model you have the following settings for Initial Head:



- Use Specified Heads will use the values that are defined for "Initial Heads" at the Define Properties step.
- Use Ground Elevation will use the elevation values for the top of Layer 1.
- Use Previous MODFLOW Run requires you to select a .HDS file from a previous MODFLOW Run and specify the Time step to be used.

Select previous HDS file	-	□ ×
Previous HDS File		Browse
Time step		
	<u>0</u> K	<u>C</u> ancel



The selected .HDS file cannot be the same as the .HDS file in the current translation directory. If you select Use .HDS from Previous MODFLOW Run option, you must choose a .HDS file from another directory.

11.8.1.3 Output Control

The Output Control run options set the information and frequency of information written and saved to the various MODFLOW-USG output files (see the following figure).

FLOW-USG				5	Save to bina	ry		Print t	to .LST	
3	End Time	Stress Period	Time Step	Heads	DDown	F.Term	Heads	DDown	F.Term	Budget
	19.55	1	1							
	43.013	1	2		Π		Π		Π	
	71.17	1	3	Π	Π		Π	Π		
	104.95	1	4		Π		Π			
	145.49	1	5		Π		Π		Π	
	194.14	1	6	Π	Π		Π		Π	
	252.52	1	7	Π	Π		Π	Π	Π	$\mathbf{\nabla}$
	322.58	1	8		Π		Π		Π	
	406.65	1	9	Π	Π		Π	Π		
	507.53	1	10		Π		Π		Π	
	628.58	1	11	Π	Π			Π		
	773.85	1	12		Π					
	948.17	1	13							\triangleleft
	1157.36	1	14		Π		Π		Π	
	1408.38	1	15				Π			
	1709.61	1	16							
	2071.084	1	17							
	2504.85	1	18		Π					\triangleleft
	3025.37	1	19		Π					
	3650	1	20				Π	Π		

Each MODFLOW simulation can produce three binary output files and one ASCII output file:

- Binary head file (modelname.HDS)
- Binary drawdown file (modelname.DDN)
- Binary cell-by-cell flow/budget file (modelname.CBC)
- ASCII listing file (modelname.LST)

The binary files contain head, drawdown, and flow exchange values for each grid cell, while the ASCII listing file contains all relevant information on the operation of MODFLOW-USG, and the simulation results. The listing (.LST) file is useful if errors occur during a simulation and you want to know how far MODFLOW-USG progressed, or if you want to examine head or drawdown values at given intervals.

For a steady-state simulation, only one set of values for each grid cell are written to these files. However, for transient simulations, each grid cell may contain simulation results for every time step within a given stress period, resulting in files that can become unnecessarily large. By default, the information is saved in the binary files at the end of each stress period and at the end of the simulation in the listing (.LST) file. Note that the cell-by-cell flows are saved by default for each time step if ZoneBudgetUSG or MOD-PATH3DU are included in the simulation.

The first two columns list the available stress periods and associated time steps for the entire simulation (only one stress period and time step will be listed for steady-state simulations). The remaining columns indicate the information which can be written and saved to the various MODFLOW output files. To select an output option, click in the appropriate checkbox and a checkmark (\bowtie) will appear to indicate that the selected information will be written for the selected time step.

The columns labeled Save to Binary will save the output information to the binary files as described below.

- Heads: Saves the heads in the binary heads file (.HDS).
- DDown: Saves the drawdown in the binary drawdown file (.DDN).
- F.Term: Saves the cell-by-cell flow terms in the binary budget (.CBC) file.

Please Note: The Zone Budget program uses the CBC file for calculating the flow between zones. Therefore, to change the frequency at which the Zone Budget information is saved, select the desired F.Term intervals saved to binary.

The columns labeled Print to .LST will save the output information to the listing file as described below.

- Heads: Saves the heads in the listing file.
- **DDown**: Saves the drawdown in the listing file.
- F.Term: Saves the flux terms (cell by cell flow terms) in the listing file.
- Budget: Saves the budget information in the listing file.

Please Note: MODFLOW only allows the flow terms (F.Term) to be stored once, in either the binary budget file (.CBC) or the listing file (.LST). Be aware that this setting can be lost if MODFLOW-USG is being run together with MOD-PATH3DU, because MOD-PATH3DU requires the flow terms to be written to the .CBC file, and not to the .LST file.

Saving Output Every Nth Time Step

For simulations with many stress periods and time steps, it can be very tedious to manually select the desired output time step intervals. The row of fields underneath the Output Control table are used to specify regular time step intervals for saving files during Each N-th step in each stress period. The first text box is where the N value is entered. To apply this value to the column, click the underlying checkbox.

If a subsequent engine is included in the run formation (e.g. ZoneBudgetUSG, MOD-PATH3DU) with the MODFLOW-USG simulation, Visual MODFLOW Flex will save the flow terms for all time steps by default.

11.8.1.4 Advanced Settings

Advanced translation settings are available for flow simulations to enable more advanced control of translation and package settings. General and package-specific advanced settings are described below. General advanced settings are available for all Flow and Transport engines supported by Visual MODFLOW Flex, while certain engines have additional package-specific advanced settings available:

- <u>General</u>
- MODFLOW-USG

Advanced Settings - General

The following settings are available for all packages:

~	General				
	CUnit	0			
	Ext	.BAS			
	LUnit	10			
	Run	Yes			
	Translate	Yes			

- CUnit: The index for the package in the CUNIT array of the BAS file [read-only]
- Ext: The file extension of the package [read-only]
- LUnit: The file unit number to which the package will be read/written during the engine run [read-only]
- **Run**: Yes/No switch to determine whether the package will be added to the .NAM/.IN file and run during the simulation. **Note**: certain packages are required as part of a simulation (e.g. BAS file) and must always be run the run option for these packages is disabled.
- **Translate**: Yes/No switch to determine whether the package will be translated. **Note**: packages that do not have sufficient data will not be translated (e.g. a river package file will not be translated if no rivers are listed in the model explorer in the active numerical model workflow).

Please Note: If a supported package is *not* represented in the model, by default it will not be translated and run, even if translate and run are both set to "Yes". For example if there are no drains represented in the model, then the DRN package will not be translated and run.

Working with Custom/Externally Developed Input Package Files

If you develop or modify a package input file outside of Visual MODFLOW Flex, you can still use it as part of your modeling workflow within the Flex environment. This is particularly useful if you want to use one or more packages that are not yet supported in Visual MODFLOW Flow or if you have custom methods/utilities to generate input files. To use a custom input file:

- 1. Set Run = Yes
- 2. Set Translate = No
- Add the input file to the model run folder with the correct name and extension: [model].[ext]. The model run folder can be found by selecting the folder icon button [
], the model name will correspond to the name of your conceptual model, and the extension will be the Ext value for the package in question. For example, if you will to run the drain return package (DRT), and you are running a model where:
 - the Visual MODFLOW Flex project file is called SiteModel.amd,
 - the Conceptual Model is called Concept1,
 - the Grid is called NumericalGrid,
 - the Run is called Run 1, and
 - the Flow Engine is MODFLOW-2005

Then the DRT file must be saved as:

.\SiteModel.data\MODFLOW\NumericalGrid\Run1\MODFLOW-2005\Concept1.DRT

If the above conditions are met, the custom package file will inserted into the relevant .NAM/ .IN file and run with the model. Note that certain results from unsupported packages will not be read back into Visual MODFLOW Flex, such as the flow balance terms associated with the SFR package.

Advanced Settings - MODFLOW-USG

Package-specific settings for MODFLOW-USG are described below:

OC Settings

The following settings are specific to the Output Control (OC) package:

\sim	UC C				
	Output control file format type	Use keywords			
	Use compact budget	Yes			

- Output control file format type An integer value used to define which cell in a vertical column that recharge and discharge is simulated.
 - use codes the output control file will be generated with integer codes to that mark what output will be generated for each time step
 - use keywords [Default] the output control file will be generated with keywords that are more easily legible. This option also enables the use of the compact budget format.
- Use compact budget an optional keyword that controls the format of the output binary file
 - Yes [Default] the compact budget format will be used. This format uses less disk space than the standard format developed with MODFLOW-88
 - \circ No the standard format developed with MODFLOW-88 will be used.

CHD Settings

The following settings are specific to the specified head (CHD) package:

 Misc Duplicate CHD Cell Filter

Average

- **Duplicate CHD Cell Filter** In some cases, multiple constant head cells may be assigned to the same cell, particularly when working with conceptual models. When MODFLOW formulates the system of equations to be solved, it simply sequentially adds boundary condition terms to the matrix and/or solution vector for all other boundary conditions this is usually not a problem as these values still require a head solution for that cell; however adding the constant head values together typically does not produce the intended (i.e. without intervention, overlapping constant head boundary conditions in the same cell with values of 201 and 199 would result in an output head value at that cell of 400, which is most likely an undesired result). Therefore, Visual MODFLOW Flex includes an optional filter to handle these cases on translation:
 - Minimum the minimum specified head value for the current stress period in the cell(s) with multiple values will be assigned
 - Maximum the maximum specified head value for the current stress period in the cell(s) with multiple values will be assigned
 - Average [Default] the arithmetic mean of specified head values for the current stress period in the cell(s) with multiple values will be assigned
 - Sum specified head values values for the current stress period in the cell(s) with multiple values will be added.

GNC Settings

The following settings are specific to the ghost-node correction package:

\mathbf{v}	GNC	
	I2Kn	0 - Do not apply second-order correction
	ISYMGNCn	0 - Use implicit update for asymmetric formulation

• **I2KN** - a flag indicating if second-order correction is also applied to the unconfined transmissivity term by using the smoothed function for expressing the downstream

node head for "flow-to-dry-cell" option (h) to compute the transmissivity of the ghost node instead of using h.

- o 0 Do not apply second order correction [Default]
- o 1 Apply second order correction
- **ISYMGNCn** a flag indicating if the GNC formulation is applied in an implicit manner on the left-hand side matrix for an asymmetric system, or in an explicit manner on the right-hand side vector with iterative updates as is required for symmetric systems.
 - $\,\circ\,$ 0 Use implicit update for asymmetric formulation [Default]
 - $\,\circ\,$ 1 Use explicit update for asymmetric formulation

11.8.2 MODFLOW-6

This chapter describes the features, functionality, and options in the Translation section of the Visual MODFLOW Flex interface when using MODFLOW-6 to perform the groundwater flow (GWF) simulation. The Translation section is where the MODFLOW-6 packages are generated.

Depending on the <u>Modeling Objectives</u> and if MODFLOW-6 is selected at the <u>Single Run</u> step (and associated options), the main items under the translation tree will include MODFLOW-6 and/or MODFLOW-6 <u>Transport</u>.

If you are not familiar with MODFLOW-6 and how it has been implemented in Visual MODFLOW Flex, it is <u>strongly</u> <u>recommended</u> that you familiarize yourself with the MODFLOW-6 framework and input file structure, particularly if you intend to use some of the advanced features available in MODFLOW-6 and/or you wish to work with the input files directly.

At a minimum, please read <u>Introduction to MODFLOW-6</u> and the subtopics in the present section.

MODFLOW-6 Groundwater Flow Model Settings:

- General
- MODFLOW-6 Settings
- Solver Settings
- Initial Heads
- Output Control
- Advanced Settings

11.8.2.1 Introduction to MODFLOW-6

MODFLOW-6 is the latest core version of MODFLOW and represents the consolidation of a number of features that were available in separate engines, including:

- Unstructured grids (MODFLOW-USG),
- Newton-Raphson formulation (MODLFOW-NWT),
- Dual-domain solute transport (MT3D-MS),
- Multiple nested model grids (MODFLOW-LGR),
- Density-dependent flow and solute transport (SEAWAT)

as well as some new/unique features:

- full 3D anisotropy tensor support (via the XT3D formulation),
- multiple stress package instances, and
- mover/exchange packages

Note that not all of these features are supported in the latest version of Visual MODFLOW Flex; however, we will add support (based on user demand). If there is a feature of MODFLOW-6 that is not yet supported that you'd like to see added in a future version of Visual MODFLOW Flex, please let us know at support@waterloohydrogeologic.com.

MODFLOW-6 versus Previous Versions of MODFLOW

Development of previous versions of MODFLOW (e.g. MODFLOW-2000, MODFLOW-2005, MODFLOW-NWT, SEAWAT, MODFLOW-SURFACT, and MODFLOW-USG) was largely incremental in such a way that input file structure were largely consistent across versions or only required modest changes to the input structure of some input package files. Unlike these previous versions, MODFLOW-6 was completely re-written by the United States Geologic Survey staff and collaborators. As part of the re-write, the entire framework and associated structure of the input/output files are significantly different. The new input file structure is based on a pseudo-object oriented paradigm that uses keywords and a multi-model/multi-solution simulation framework. This generally makes the files more human readable; however, these changes mean that files from previous versions are not compatible with MODFLOW-6.



It is <u>strongly recommended</u> that you familiarize yourself with the MODFLOW-6 framework and input file structure, particularly if you intend to use some of the advanced features available in MODFLOW-6 and/or you wish to work with the input files directly.

Working with MODFLOW-6 in Visual MODFLOW Flex

This section highlights important differences and considerations for working MODFLOW-6 as compared to previous versions:

- MODFLOW-6 Input file formats: as described in the inset above, the input files for MODFLOW-6 are completely different from previous versions of MODFLOW. Although many of the same package names apply between previous versions of MODFLOW and MODFLOW-6, the input structures are different and in some cases packages have been replaced and/or the location of input variables has been moved into new or different packages. For example, the BAS package in older versions of MODFLOW included information about the (in)active status of grid cells (IBOUND) and starting head values (SHEAD); however, MODFLOW-6 no longer has a BAS package grid cell status information has been included in the DIS(V) package (IDOMAIN) and the starting heads have been moved to the IC package. For more details, please refer to the input documentation for more details (USGS, <u>2022</u>).
- MODFLOW-6 Simulations: the MODFLOW-6 framework includes a new simulation level structure - this allows modelers to develop flow (and transport models) of groundwater systems in a hierarchical manner that can incorporate one or more models of the same of different types. Currently, only groundwater flow (GWF) and groundwater transport (GWT) type models are supported and the current version of Visual MODFLOW Flex has a further limitation that only one groundwater flow model and separate, but linked transport models for each species may be included in the simulation.
- Time Discretization: MODFLOW-6 includes the time discretization (TDIS) package and requires that time be discretized at the simulation level - that is information about temporal control, such as the number and duration of stress periods, the number time steps and associated multipliers are specified for the simulation as a whole rather than for each GWF/GWT model individually. This means that stress periods and time steps should be specified in a way that is suitable for all models in the simulation. If included, transport simulation typically requires finer discretization of time steps due to numerical issues associated with solving the advection-dispersion equation as reflected in the dimensionless Courant number ($C_r = v_i \Delta t / \Delta x_i$, where is v_i is the groundwater velocity in a given direction, Δt is the time step, and Δx_i is the grid spacing in that direction). Special care should be taken with selecting time steps - Courant numbers of 2 and generally no more than 5 are commonly recommended for problems involving solute transport.
- **Multi-species Transport**: MODFLOW-6 currently only supports single species transport GWT models; however, multi-species modeling in a single simulation is possible by adding a separate groundwater transport (GWT) model for each solute/species to the simulation. The GWT model does not currently support kinetic reactions between species in separate models.
- **Transport Boundary Conditions**: in Visual MODFLOW Flex, the default species concentrations for boundary conditions is set to -1; which previous transport engines such as MT3D-MS, RT3D, and SEAWAT interpret as zero concentrations for sources and ambient concentrations for sinks, which is particularly useful for multi-species

simulation with boundary conditions where only a subset of the species have known/specified concentrations. MODFLOW-6 does not include this interpretation (likely since species concentrations are modeled independently). Currently Visual MODFLOW Flex supports transport sources/sinks in boundary conditions using AUXILIARY variables in each boundary condition along with the SSM package. To minimize discrepancies between the engines, Visual MODFLOW Flex will treat transport boundary conditions as follows during MODFLOW-6 translation:

- If ALL concentrations of a given species in a boundary condition are negative, the boundary condition package in the GWF will omit that species as an AUXILIARY variable and omit that boundary from the SSM file in the GWT model that corresponds to that species
- If ANY concentrations of a given species in a boundary concentrations are greater than or equal to 0, then the boundary condition package in the GWF model will include that species as an AUXILLIARY variable and include the boundary condition in the SSM package in the GWT for that species. In this case, negative concentrations should be set to zero or the boundary condition should be split into two separate boundary conditions: one will all negative concentrations and one with all non-negative concentrations.

The exception for this is the Mass Source Loading package, which is designed to simulate solute mass fluxes that are positive (e.g. a source zone, spill, etc.) or negative (e.g. an in-situ treatment zone).

There are many more differences than those listed above, please consult the references listed below for more details and refer to the other topics in this Section about MODFLOW-6.

Recommended Reading

The following resources may be useful for learning more about MODFLOW-6:

Official USGS MODFLOW-6 Website: <u>https://www.usgs.gov/software/modflow-6-usgs-modular-hydrologic-model</u>

Documentation:

- Hughes, J.D., Langevin, C.D., and Banta, E.R., 2017, <u>Documentation for the</u> <u>MODFLOW 6 framework</u>: U.S. Geological Survey Techniques and Methods, book 6, chap. A57, 40 p., <u>https://doi.org/10.3133/tm6A57</u>.
- Langevin, C.D., Hughes, J.D., Banta, E.R., Niswonger, R.G., Panday, Sorab, and Provost, A.M., 2017, <u>Documentation for the MODFLOW 6 Groundwater Flow Model</u>: U.S. Geological Survey Techniques and Methods, book 6, chap. A55, 197 p., <u>https://doi.org/10.3133/tm6A55</u>.
- Langevin, C.D., Provost, A.M., Panday, Sorab, and Hughes, J.D., 2022, <u>Documentation for the MODFLOW 6 Groundwater Transport Model</u>: U.S. Geological Survey Techniques and Methods, book 6, chap. A61, 56 p., <u>https://doi.org/10.3133/tm6A61</u>.

 United States Geological Survey, 2022. <u>MODFLOW-6 - Description of Input and</u> <u>Output (Version 6.4.1)</u>. United States Geological Survey, Water and Science Availability and Use Science Program, MODFLOW 6 Development Team. Dec 2022.

11.8.2.2 MODFLOW-6 Settings

The following settings are available for the MODFLOW-6 flow engine:

Run Type: Steady-State or Transient

If the Steady-State Flow option is selected, Visual MODFLOW Flex will prepare the data set for a steady-state flow simulation, and will automatically use the data from the first time period (only) of each boundary condition and pumping well defined in Visual MODFLOW Flex to run the model to achieve flow equilibrium (i.e. a time-independent solution since all inputs are constant).

Please Note: if running a steady-state model, at least one boundary condition with a head of known elevation must be specified (e.g. constant head, river stage, drain bottom, or general head elevation).

If the Transient Flow option is selected, Visual MODFLOW Flex will prepare the data set for a transient flow simulation. During this process, Visual MODFLOW Flex will automatically merge all of the different time period data defined for each pumping well and boundary condition into the stress period format required by MODFLOW-6. This creates a time-dependent flow solution, as the model is being run with different inputs at different times.

Steady-State Simulation Time: specified time for the mass balance terms in a steady-state run.

Please Note: the settings for Property Package and Save .FLO file available for other flow engines are not applicable for MODFLOW-6. MODFLOW-6 only has one property package - the node property flow (NPF) package and the .FLO file is not necessary for MODFLOW-6 as transport as the link between flow and transport is handled through the flow model interface when running flow and transport models sequentially or through exchange package(s) if running a coupled flow and transport simulation.

١	🔄 🗇 🤤 💿		
	Settings Translation Log		
	🖃 General	✓ General	
ł	Settings	Run Type	Steady-State
ł	MODFLOW-6	Steady-State Simulation Time	1
ł			
ł			
ł			
ł			
ł	Advanced Settings		
ł			
ł			
ł			
ł		Simulation Type: Steady-State or Transient	
ł			
	Settings Solvers Initial Heads Output Control Advanced Settings	Run Type Simulation Type: Steady-State or Transient	

Stress Periods and Time Steps

The Time Steps option is only available when you are running a transient model (i.e. when Transient Flow run type is selected). For transient flow simulations, Visual MODFLOW Flex will automatically merge all of the different time periods defined for all of the different pumping wells and boundary conditions into the uniform stress period format required by MODFLOW. A stress period is defined as a time period in which all the stresses (boundary conditions, pumping rates, etc.) on the system are constant. Unfortunately, the data collected for each modeling site is rarely synchronized in terms of stress periods, so Visual MODFLOW Flex merges the time schedules for all pumping wells and boundary conditions to determine the length of each stress period for a transient simulation. As a result, the user cannot directly modify the number of stress periods or the length of each stress period.

The Time step options window (as shown in the following figure) is used to define the number of Time steps in each stress period and the time step Multiplier is used to increment each time step size.

General Settings MODFLOW-6 Settings Solvers Initial Heads Output Control ∂. Advanced Settings	✓ General Run Type Steady-State Simu	ilation Time		Transient 1		
	Run Type Simulation Type: Stead	dy-State or Transien	t			
	Time Steps Value	Start	End	Time Steps	Multiplier	Steady-State
	Stress Period	Start	End	Time Steps	Multiplier	Steady-State
	Stress Period	0.000	End 31.000	10	1.2	
	Stress Period 1 2	0.000 31.000	End 31.000 60.000	10 10	1.2 1.2	
	Stress Period 1 2 3	0.000 31.000 60.000	End 31,000 60,000 91,000	10	1.2 1.2 1.2	
	Stress Period 1 2 3 4	0.000 31.000 60.000 91.000	End 31.000 60.000 91.000 121.000	10 10 10	1.2 1.2 1.2 1.2 1.2	
	Stress Period 1 2 3 4 5	0.000 31.000 60.000 91.000 121.000	End 31.000 60.000 91.000 121.000 152.000	10 10 10 10	1.2 1.2 1.2	
	Stress Period 1 2 3 4	0.000 31.000 60.000 91.000	End 31.000 60.000 91.000 121.000	10 10 10 10 10 10	1.2 1.2 1.2 1.2 1.2 1.2	
	Stress Period 1 2 3 4 5 6	0.000 31.000 60.000 91.000 121.000 152.000	End 31.000 60.000 91.000 121.000 152.000 182.000	10 10 10 10 10 10 10	12 12 12 12 12 12 12 12 12	
	Stress Period 1 2 3 4 5 6 7	0.000 31.000 60.000 91.000 121.000 152.000 182.000	End 31.000 60.000 91.000 121.000 152.000 182.000 213.000	10 10 10 10 10 10 10 10	12 12 12 12 12 12 12 12 12	
	Stress Period 1 2 3 4 5 6 7 8	0.000 31.000 60.000 91.000 121.000 152.000 182.000 213.000	End 31.000 60.000 91.000 121.000 152.000 182.000 213.000 244.000	10 10 10 10 10 10 10 10 10	1.2 1.2 1.2 1.2 1.2 1.2 1.2 1.2 1.2 1.2	
	Stress Period 1 2 3 4 5 6 7 8 9	0.000 31.000 60.000 91.000 121.000 152.000 182.000 213.000 244.000	End 31.000 60.000 91.000 121.000 152.000 182.000 213.000 244.000 274.000	10 10 10 10 10 10 10 10 10 10	1.2 1.2 1.2 1.2 1.2 1.2 1.2 1.2 1.2 1.2 1.2 1.2 1.2 1.2	

The Stress Period column indicates the stress period number while the Start and End columns indicate the start time and end time, respectively, for each stress period.

Each stress period is divided into a user-defined number of Time steps whereby the model will calculate the head solution at each time step. The default value for Time steps is 10.

The time step Multiplier is the factor used to increment the time step size within each stress period (i.e. it is the ratio of the value of each time step to that of the preceding time step). The default value is 1.2. A time step Multiplier value greater than 1 will produce smaller time steps at the beginning of a stress period resulting in a better representation of the changes of the transient flow field. Thus increasing the number of time steps in a simulation may result in smoother head or drawdown versus time curves.

The steady-state column indicates if the stress period is transient or steady-state. This setting allows individual stress periods in a single simulation to be either transient or steady state instead of requiring the entire simulation to be either steady state or transient. Steady-state and transient stress periods can occur in any order. Commonly the first stress period may be run as steady state, to produce a solution that is used as the initial condition for subsequent transient stress periods.

Accommodating Boundary Conditions with Varying End Times

Visual MODFLOW Flex allows you to define boundary conditions with varying end times; the number of stress periods for the model will be calculated from the end time of the longest boundary condition. If there is a stress period where there are no data defined for a boundary condition, then you will see an entry of "0" in the appropriate package, for that stress period; this denotes that zero cells are defined for that stress period. In the case of pumping wells, you will see a rate of 0 for the well cells.

11.8.2.3 Solver Settings

Solvers in MODFLOW-6 are handled through the iterative model solution (IMS) package which is used to solve flow and/or transport simulations. The IMS package uses a linear and non-linear methods to solve the simultaneous equations produced by the model(s) as described below:

ings Translation Log nam T	DIS	IMS	DIS	IC	OC	NPF	CHD	CHD(2)	RIV	WEL	STO	nam(2)
General	~	Gene	_									
Settings		Selecte	ed Solve	er 👘				ltera	tive M	atrix So	lver (IN	AS)
MODFLOW-6												
Settings												
Solvers Initial Heads												
Output Control	~	Option	าร									
Advanced Settings		PrintOp						Nor				
MODFLOW-6 Transport-Specific		Comple						Sim				
General			terOutpu					Fals				
Solvers			erOutpu	t				Fals				
Initial Concentrations		NoPtc						Firs	-			
Output Control		AtsOut		umFracti	on			0.2	5			
	 ~		r aximum					100				
		InnerD						1E-				
		InnerR						1E-				
			Accelera	tion					GStab			
		Relaxa	tionFact	or				0				
		Precon	ditionerl	Levels				0				
		Precon	ditioner	Drop Tole	rance			0				
		Numbe	rOrthog	onalizatio	ns			0				
		Scaling	Method					Nor	ne			
			ringMet	hod				Nor	ne			
	~	Nonlir										
			VClose					0.0	-			
			laximum					100				
			Relaxatio					Nor				
				nGamma	3			0.2				
				on Theta on Kappa				0.7				
				on Kappa on Momen	tum.			0.0				
			ackingN		lum			10	01			
			-	olerance				100	00			
			-	eduction	Factor			0.2				
			-	esidualLi				100				
	PrintOption											
	Af	ag that (controls					rom the sol				
	me	ans print	nothing	. SUMM	ARY mea	ans print o	only the to	tal number	of iterat	ions and		
								trix solver o convergen				

General Solution Options

The following settings are optional in the IMS package:

- **PrintOption**: An optional keyword setting that determines the print level of the solver in the listing file:
 - Summary means print only the total number of iterations and nonlinear residual reduction summaries.
 - All means print linear matrix solver convergence information to the solution listing file and model specific linear matrix solver convergence information to each model listing file in addition to *Summary* information.
 - None means that no solver information will be printed. This is the default option.
- **Complexity**: is an optional keyword that defines default non-linear and linear solver parameters.

- Simple indicates that default solver input values will be defined that work well for nearly linear models. This option is generally suitable for models that do not include nonlinear stress packages and models that are either confined or consist of a single unconfined layer that is thick enough to contain the water table within a single layer.
- Moderate: indicates that default solver input values will be defined that work well for moderately nonlinear models. This option is generally suited for models that include nonlinear stress packages and models that consist of one or more unconfined layers. The *Moderate* option should be used when the *Simple* option does not result in successful convergence.
- Complex: indicates that default solver input values will be defined that work well for highly nonlinear models. This option is generally suited for models that include nonlinear stress packages and models that consist of one or more unconfined layers representing complex geology and surface-water/groundwater interaction. The complex option should be used when the moderate option does not result in successful convergence.
- Custom: indicates that custom values will be defined for the linear and non-linear solvers.

If the Simple, Moderate, or Complex options are selected, then only the items in the linear and non-linear solver sections below marked with * will be translated. All other options will use the defaults below:

SETTINGS		COMPLEXITY	
SETTINGS	SIMPLE	MODERATE	COMPLEX
NON-LINEAR SOLVER SE	TTINGS		
OUTER_DVCLOSE *	0.001	0.01	0.1
OUTER_MAXIMUM *	25	50	100
UNDER_RELAXATION	NONE	DBD	DBD
UNDER_RELAXATION_TH ETA	1	0.9	0.8
UNDER_RELAXATION_KA PPA	0	0.0001	0.0001
UNDER_RELAXATION_G AMMA	0	0	0
UNDER_RELAXATION_M OMENTUM	0	0	0
BACKTRACKING_NUMBE R	0	0	20
BACKTRACKING_TOLER ANCE	0	0	1.05

BACKTRACKING_REDUC TION_FACTOR	0	0	0.1		
BACKTRACKING_RESIDU AL_LIMIT	0	0	0.002		
LINEAR SOLVER SETTINGS					
INNER_MAXIMUM *	50	100	500		
INNER_DVCLOSE *	0.001	0.01	0.1		
INNER_RCLOSE *	0.1	0.1	0.1		
RCLOSE_OPTION	infinity-norm	infinity-norm	infinity-norm		
LINEAR_ACCELERATION	CG	BICGSTAB	BICGSTAB		
RELAXATION_FACTOR	0	0.97	0		
PRECONDITIONER_LEVE LS	0	0	5		
PRECONDITIONER_DRO P_TOLERANCE	0	0	0.0001		
NUMBER_ORTHOGONALI ZATIONS	0	0	2		
SCALING_METHOD	NONE	NONE	NONE		
REORDERING_METHOD	NONE	NONE	NONE		

- **CsvOuterOutput**: if this option is set to yes, then outer iteration convergence information will be written to a comma separated values file in the GWF subfolder. This option is off by default. Information written to this file includes maximum dependent-variable (for example, head or concentration) change convergence information at the end of each outer iteration for each time step.
- **CsvInnerOutput**: if this option is set to yes, then inner iteration convergence information will be written to a comma separated values file in the GWF subfolder. This option is off by default. Information written to this file includes maximum dependent-variable (for example, head or concentration) change and maximum residual convergence information for the solution and each model (if the solution includes more than one model) and linear acceleration information for each inner iteration.
- NoPTC: is a settings that is used to control the pseudo-transient continuation (PTC) options for steady state periods for models using the Newton-Raphson formulation (which is controlled by in NAM file <u>settings</u>):
 - o None: PTC will not be used in solution
 - o First: PTC will be activated for the first stress period
 - o All: PTC will be deactivated for all stress periods

For many problems, PTC can significantly improve convergence behavior for steadystate simulations, and for this reason it is active by default. In some cases; however, PTC can worsen the convergence behavior, especially when the initial conditions are similar to the solution. When the initial conditions are similar to (or exactly the same as) the solution and convergence is slow, then the NO_PTC FIRST option should be used to deactivate PTC for the first stress period. The NO_PTC ALL option should also be used in order to compare convergence behavior with other MODFLOW versions, as PTC is only available in MODFLOW 6.

• AtsOuterMaximumFraction: real value defining the fraction of the maximum allowable outer iterations used with the Adaptive Time Step (ATS) capability if it is active. If this value is set to zero by the user, then this solution will have no effect on ATS behavior. This value must be greater than or equal to zero and less than or equal to 0.5 or the program will terminate with an error. If it is not specified by the user, then it is assigned a default value of one third. When the number of outer iterations for this solution is less than the product of this value and the maximum allowable outer iterations, then ATS will increase the time step length by a factor of DTADJ in the ATS input file. When the number of outer iterations for this solution is greater than the maximum allowable outer iterations, then ATS (if active) will decrease the time step length by a factor of 1 / DTADJ.

Non-Linear Solver Options

The following settings are available for the Non-linear solver:

- OUTER_DVCLOSE: real value defining the dependent-variable (for example, head or concentration) change criterion for convergence of the outer (nonlinear) iterations, in units of the dependent-variable (for example, length for head or mass per length cubed for concentrations). When the maximum absolute value of the dependent-variable change at all nodes during an iteration is less than or equal to OUTER_DVCLOSE, iteration stops.
- **OUTER_MAXIMUM**: integer value defining the maximum number of outer (nonlinear) iterations. For a linear problem OUTER_MAXIMUM should be 1.
- UNDER_RELAXATION: an optional keyword that defines the nonlinear underrelaxation schemes used. Under-relaxation is also known as dampening, and is used to reduce the size of the calculated dependent variable before proceeding to the next outer iteration. Under-relaxation can be an effective tool for highly nonlinear models when there are large and often counteracting changes in the calculated dependent variable between successive outer iterations. By default under-relaxation is not used.
 - o NONE [Default] under-relaxation is not used
 - SIMPLE Simple under-relaxation scheme with a fixed relaxation factor (under relaxation gamma (see below)) is used.
 - o COOLEY Cooley under-relaxation scheme is used.
 - o DBD delta-bar-delta (DBD) under-relaxation is used.

Note that the under-relaxation schemes are often used in conjunction with problems that use the Newton-Raphson formulation (which is controlled by in NAM file <u>settings</u>); however, experience has indicated that they also work well for non-Newton problems, such as those with the wet/dry options of MODFLOW 6.

- UNDER_RELAXATION_GAMMA: a real value defining either the relaxation factor for the simple complexity scheme or the history or memory term factor of the Cooley and delta-bar-delta algorithms. For the simple scheme, a value of one indicates that there is no under-relaxation and the full head (or concentration) change is applied. This value can be gradually reduced from one as a way to improve convergence; for well behaved problems, using a value less than one can increase the number of outer iterations required for convergence and needlessly increase run times. Under relaxation gamma must be greater than zero for the simple scheme or the program will terminate with an error. For the Cooley and delta-bar-delta schemes, Under relaxation gamma is a memory term that can range between zero and one. When Under relaxation gamma is zero, only the most recent history (previous iteration value) is maintained. As Under relaxation gamma is increased, past history of iteration changes has greater influence on the memory term. The memory term is maintained as an exponential average of past changes. Retaining some past history can overcome granular behavior in the calculated function surface and therefore helps to overcome cyclic patterns of non-convergence. The value usually ranges from 0.1 to 0.3; a value of 0.2 works well for most problems. Under relaxation gamma is only used in the simulation if Under relaxation is not None.
- UNDER_RELAXATION_THETA: a real value defining the reduction factor for the learning rate (underrelaxation term) of the delta-bar-delta algorithm. The value of *under relaxation theta* is between zero and one. If the change in the dependent-variable (for example, head or concentration) is of opposite sign to that of the previous iteration, the under-relaxation term is reduced by a factor of *under relaxation theta*. The value usually ranges from 0.3 to 0.9; a value of 0.7 works well for most problems. *Under relaxation theta* is only used in the simulation if *under relaxation* is DBD.
- UNDER_RELAXATION_KAPPA: a real value defining the increment for the learning rate (under-relaxation term) of the delta-bar-delta algorithm. The value of *under relaxation kappa* is between zero and one. If the change in the dependent-variable (for example, head or concentration) is of the same sign to that of the previous iteration, the under-relaxation term is increased by an increment of *under relaxation kappa*. The value usually ranges from 0.03 to 0.3; a value of 0.1 works well for most problems. *Under relaxation kappa* is only used in the simulation if *under relaxation* is DBD.
- UNDER_RELAXATION_MOMENTUM: a real value defining the fraction of past history changes that is added as a momentum term to the step change for a nonlinear iteration. The value of *under relaxation momentum* is between zero and one. A large momentum term should only be used when small learning rates are expected. Small amounts of the momentum term help convergence. The value usually ranges from 0.0001 to 0.1; a value of 0.001 works well for most problems. *Under relaxation momentum* is only used in the simulation if *under relaxation* is DBD.
- **BACKTRACKING_NUMBER**: an integer value defining the maximum number of backtracking iterations allowed for residual reduction computations. If *backtracking*

number = 0 then the backtracking iterations are omitted. The value usually ranges from 2 to 20; a value of 10 works well for most problems.

- **BACKTRACKING_TOLERANCE**: a real value defining the tolerance for residual change that is allowed for residual reduction computations. The *backtracking tolerance* value should not be less than one to avoid getting stuck in local minima. A large value serves to check for extreme residual increases, while a low value serves to control step size more severely. The value usually ranges from 1.0 to 106; a value of 104 works well for most problems but lower values like 1.1 may be required for harder problems. *Backtracking tolerance* is only used in the simulation if *backtracking number* is greater than zero.
- **BACKTRACKING_REDUCTION_FACTOR**: real value defining the reduction in step size used for residual reduction computations. The value of is between zero and one. The value usually ranges from 0.1 to 0.3; a value of 0.2 works well for most problems. *Backtracking reduction factor* is only used in the simulation if *backtracking number* is greater than zero.
- **BACKTRACKING_RESIDUAL_LIMIT**: a real value defining the limit to which the residual is reduced with backtracking. If the residual is smaller than *backtracking residual limit*, then further backtracking is not performed. A value of 100 is suitable for large problems and residual reduction to smaller values may only slow down computations. *Backtracking residual limit* is used in the simulation if *backtracking number* is greater than zero.

Linear Solver Options

The following settings are available for the Linear solver:

- **INNER_MAXIMUM**: an integer value defining the maximum number of inner (linear) iterations. The number typically depends on the characteristics of the matrix solution scheme being used. For nonlinear problems, *inner maximum* usually ranges from 60 to 600; a value of 100 will be sufficient for most linear problems.
- INNER_DVCLOSE: a real value defining the dependent-variable (for example, head or concentration) change criterion for convergence of the inner (linear) iterations, in units of the dependent-variable (for example, length for head or mass per length cubed for concentration). When the maximum absolute value of the dependent-variable change at all nodes during an iteration is less than or equal to *inner dvclose*, the matrix solver assumes convergence. Commonly, *inner_dvclose* is set equal to or an order of magnitude less than the *outer_dvclose* value specified for the non-linear block.
- **INNER_RCLOSE**: a real value that defines the flow residual tolerance for convergence of the IMS linear solver and specific flow residual criteria used. This value represents the maximum allowable residual at any single node. Value is in units of length cubed per time, and must be consistent with MODFLOW-6 length and time units. Usually a value of 0.1 is sufficient for the flow-residual criteria when meters and seconds are the defined MODFLOW-6 length and time.

∆h ≤

- RCLOSE_OPTION: an optional keyword that defines the specific flow residual criterion used.
 - STR/CT: an optional keyword that is used to specify that *inner rclose* represents a infinity-Norm (absolute convergence criteria) and that the dependent-variable (for example, head or concentration) and flow convergence criteria must be met on the first inner iteration (this criteria is equivalent to the criteria used by the MODFLOW-2005 PCG package (Hill, <u>1990</u>)).
 - L2NORM_RCLOSE: an optional keyword that is used to specify that *inner rclose* represents a L-2 Norm closure criteria instead of a infinity-Norm (absolute convergence criteria). When *L2norm rclose* is specified, a reasonable initial *inner rclose* value is 0.1 times the number of active cells when meters and seconds are the defined MODFLOW-6 length and time.
 - RELATIVE_RCLOSE: an optional keyword that is used to specify that *inner rclose* represents a relative L-2 Norm reduction closure criteria instead of a infinity-Norm (absolute convergence criteria). When *relative rclose* is specified, a reasonable initial *inner rclose* value is 1.0×10⁻⁴ and convergence is achieved for a given inner (linear) iteration when *inner dvclose* and the current L-2 Norm is ≤ the product of the *relative_rclose* and the initial L-2 Norm for the current inner (linear) iteration. If *rclose option* is not specified, an absolute residual (infinity-norm) criterion is used.
 - LINEAR ACCELERATION: a keyword that defines the linear acceleration method used by the default IMS linear solvers.
 - o CG preconditioned conjugate gradient method.
 - o BICGSTAB preconditioned bi-conjugate gradient stabilized method.
 - **RELAXATION_FACTOR**: an optional real value that defines the relaxation factor used by the incomplete LU factorization preconditioners (MILU(0) and MILUT). *Relaxation_factor* is unitless and should be greater than or equal to 0.0 and less than or equal to 1.0. *Relaxation factor* values of about 1.0 are commonly used, and experience suggests that convergence can be optimized in some cases with relax values of 0.97. A *Relaxation factor* value of 0.0 will result in either ILU(0) or ILUT preconditioning (depending on the value specified for *preconditioner levels* and/or *preconditioner drop tolerance*). By default, *relaxation factor* is zero.
 - **PRECONDITIONER_LEVELS**: an optional integer value defining the level of fill for ILU decomposition used in the ILUT and MILUT preconditioners. Higher levels of fill provide more robustness but also require more memory. For optimal performance, it is suggested that a large level of fill be applied (7 or 8) with use of a drop tolerance. Specification of a *preconditioner levels* value greater than zero results in use of the ILUT preconditioner. By default, the number of *preconditioner levels* is zero and the zero-fill incomplete LU factorization preconditioners (ILU(0) and MILU(0)) are used.
 - PRECONDITIONER_DROP_TOLERANCE: a real value that defines the drop tolerance used to drop preconditioner terms based on the magnitude of matrix entries in the ILUT and MILUT preconditioners. A value of 10⁻⁴ works well for most problems. By default, the *preconditioner drop tolerance* is zero and the zero-fill incomplete LU factorization preconditioners (ILU(0) and MILU(0)) are used.

- NUMBER_ORTHOGONALIZATIONS: an integer value defining the interval used to explicitly recalculate the residual of the flow equation using the solver coefficient matrix, the latest dependent/variable (for example, head or concentration) estimates, and the right hand side. For problems that benefit from explicit recalculation of the residual, a number between 4 and 10 is appropriate. By default, the *number of orthogonalizations* is zero.
- SCALING_METHOD: an optional keyword that defines the matrix scaling approach used. By default, matrix scaling is not applied.
 - o NONE [Default] no matrix scaling applied.
 - DIAGONAL symmetric matrix scaling using the POLCG preconditioner scaling method in Hill (<u>1990</u>).
 - o L2NORM symmetric matrix scaling using the L-2 Norm.
- **REODERING_METHOD**: an optional keyword that defines the matrix reordering approach used. By default, matrix reordering is not applied.
 - o NONE [Default] original ordering.
 - o RCM reverse Cuthill McKee ordering.
 - o *MD* minimum degree ordering.

11.8.2.4 Initial Heads

In Visual MODFLOW Flex, the Initial Heads are defined at the stage of Defining the Properties. For more details, please see the section on setting <u>Initial Heads</u> in the Define Properties workflow step.

When translating your model you have the following settings for Initial Head:

🔄 🗖 G 😡		
Settings Translation Log		
	✓ General	
Settings	Initial head options	Use Ground Elevation
	Previous MODFLOW Run HDS file	C:\Users\Public\Documents\Visual MODFLOW Flex\Tutoria
···· Settings		
Solvers		
Initial Heads		
Output Control		
Advanced Settings		
	Initial head options	
	Elevation will use the elevation values for the or a previous MODFLOW Run. Warning: The se directory. If you select this option, you must chu	re defined for "Initial Heads" at the Define Properties step. Use Ground fl layer 1. Use Previous MODFLOW Run requires you to select a. HDS file from lected. HDS file cannot be the same as the .HDS file in the current translation pose a .HDS file from another directory. Or make a copy of the .HDS file from g. Model_InitialHeads.HDS), and choose this file.

- Use Specified Heads will use the values that are defined for "Initial Heads" at the Define Properties step.
- Use Ground Elevation will use the elevation values for the top of Layer 1.
- Use Previous MODFLOW Run requires you to select a .HDS file from a previous MODFLOW Run and specify the Time step to be used. The .HDS file must be based

on the same grid type and number of cells in each applicable dimension (i.e. layer, row, and columns for a structured grid, and same number of layers and cells per layer for an unstructured grid)

Select previous HDS file			x
Previous HDS File		Brows	e
Time step			
	<u>O</u> K	<u>C</u> ance	el



The selected .HDS file cannot be the same as the .HDS file in the current translation directory. If you select Use .HDS from Previous MODFLOW Run option, you must choose a .HDS file from another directory.

11.8.2.5 Output Control

Warning!

The Output Control options set the information and frequency of information written and saved to the MODFLOW-6 output files (see following figure).

Define Modeling Objectives Define Properties Define Boundary Conditions	Settings Translation Log nam	TDIS IMS I	DIS IC C	C NPF C	HD RI	(RIV(2)	WEL W	EL(2) RC	H EVT	nam(2)		
	General	Every Ntl		Heads (Sav						nam(z)		
Define Observations	a creiy rea	i step i	ineads (Sav		e to binary)							
	MODFLOW-6					Save to bin	ary	Print to .LST				
	Settings	End Time	Stress Period	Time Step	Heads	DDown	F.Term	Heads	DDown	F.Term	Budget	
Select Run Type	Solvers	1,1942	1	1								
PEST Run	Initial Heads	2 6273	1	2	П			П	П	H		
└── <mark>─</mark> Single Run Translate	Output Control	4.3469	1	3								
Run Numerical Engines	Advanced Settings	6.4105	1	4								
View Results		8.8868	1	5								
Wew Results		11.8584	1	6								
View Maps		15.4242	1	7								
a non mapo		19,7033	1	8								
		24 8382	i	9								
		31.0	1	10								
		32,1172	2	1	Π							
		33,4578	2	2								
		35.0665	2	3	П					Π		
		36,9969	2	4								
		39.3135	2	5						Π		
		42.0933	2	6	H					Η		
		45.4291	2	7								
		49.4321	2	8								
		54.2357	2	9								
		60.0	2	10	R							
		61,1942	3	1								
		67 6772	5	ว				H		H		

By default, each MODFLOW-6 groundwater flow model simulation will produce several output files as described below. The Output Control settings allow you to specify the stress period(s)/time step(s) for which model results of interest will be written to these output files. The Output Control Settings are provided in a tabular format based on the transient settings in the <u>MODFLOW-6 Settings</u> settings tab:

- Schedule:
 - End Time: the elapsed simulation time corresponding to the end of the specified stress period and time step
 - o Stress Period: the stress period in the schedule
 - o Time Step: the time step within the stress period
- Save to Binary:
 - Heads: simulated heads will be written to the binary heads file (. \GWF\modelname.HDS) for active cells in the grid for selected End Times (Stress Period/Time Step)
 - DDown: drawdown values (i.e. the simulated head minus the initial head) will be written to the binary heads file (.\GWF\modelname.DDN) for active cells in the grid for selected End Times (Stress Period/Time Step).

Please Note: when selecting drawdown output for a given End Time (Stress Period/Time Step), the head outputs must also be selected. This is due to the fact that unlike previous versions of MODFLOW, MODFLOW-6 does not produce this file natively and drawdowns are generated by Visual MODFLOW Flex as post-processing step from the output heads.

• **F. Term**: flow budget terms, sometimes called cell-by-cell and boundary condition flow terms, will be written to the binary budget file (.\GWF\modelname.BGT) for active cells and boundary conditions in the grid for selected End Times (Stress Period/Time Step). The budget information is used to generate the budget and velocity outputs in Visual MODFLOW Flex.

Please Note: for cell-by-cell values to be added to the budget file, the SAVE_FLOWS option must be enabled (set to "Yes") in the Advanced Settings for the NAM package. Similarly, for cell-to-boundary condition values to be added to the budget file, the SAVE_FLOWS option must be enabled in the Advanced Settings for each desired boundary condition. In Visual MODFLOW Flex, the SAVE_FLOWS option is enabled by default for all supported packages including the NAM file and supported boundary conditions.

- **Print to LST:** information will be written to the listing file (.\GWF\modelname.LST):
 - Heads: simulated heads will be written to the listing file for active cells in the grid for selected End Times (Stress Period/Time Step). Note that this option should be used sparingly, typically for model troubleshooting, particularly as this format can lead to overly large output files that are less efficient to work with than the binary file or related files that can be exported from Visual MODFLOW Flex.
 - F. Term: flow budget terms, sometimes called cell-by-cell and boundary condition flow terms, will be written to listing file for active cells and boundary conditions in the grid for selected End Times (Stress Period/Time Step). Note that this option should be used sparingly, typically for model troubleshooting, particularly as this format can lead to overly large output files that are less efficient to work with than the binary file or related files that can be exported from Visual MODFLOW Flex.
 - Budget: net flow budget terms, expressed at a package level, for boundary conditions and internal storage will be written to the listing file for selected End Times (Stress Period/Time Step)

Please Note: for cell-by-cell values to be added to the listing file, the PRINT_FLOWS option must be enabled (set to "Yes") in the Advanced Settings for the NAM package. Similarly, for cell-to-boundary condition values to be added to the budget file, the PRINT_FLOWS option must be enabled in the Advanced Settings for each desired boundary condition. In Visual MODFLOW Flex, the PRINT_FLOWS option is enabled by default for all supported packages including the NAM file and supported boundary conditions.

Saving Output Every Nth Time Step

For simulations with many stress periods and time steps, it can be very tedious to manually select the desired output time step intervals. The row of fields underneath the Output Control table are used to specify regular time step intervals for saving files during Each N-th step in each stress period. The first text box is where the N value is entered. To apply this value to the column, click the underlying checkbox.

If a subsequent engine is included in the run formation (e.g. ZoneBudget) with the MODFLOW simulation, Visual MODFLOW Flex will save the flow terms for all time steps by default.

11.8.2.6 Advanced Settings

Advanced translation settings are available for flow simulations to enable more advanced control of translation and package settings. General and package-specific advanced settings are described below. General advanced settings are available for all Flow and Transport engines supported by Visual MODFLOW Flex, while certain engines have additional package-specific advanced settings available:

- General
- <u>Common Options</u>
- MODFLOW-6 Flow Packages

General

The following settings are available for all packages:

✓ General		
Ext	.TDIS	
Run	Yes	
Translate	Yes	

- Ext: The file extension of the package [read-only]
- Run: Yes/No switch to determine whether the package will be added to the .NAM file and run during the simulation. Note: certain packages are required as part of a simulation (e.g. MFSIM, TDIS, IMS, NAM, IC, OC, and NPF files) and cannot be selected to not run.
- **Translate**: Yes/No switch to determine whether the package will be translated. **Note:** If a supported package is *not* represented in the model, it will not be translated and run by default, even if translate and run are both set to "Yes". For example, if there are no drains represented in the model, then the DRN package will not be translated and run.

How to Use Custom/Pre-existing Input Files
If you develop or modify a package input file outside of Visual MODFLOW Flex, you can still use it as part of your modeling workflow within the Flex environment. This is particularly useful if you want to use one or more packages that are not yet supported in Visual MODFLOW Flow or if you have custom methods/utilities to generate input files. To use a custom input file:
1. Set Run = Yes
2. Set Translate = No

- 3. Add the input file to the model run folder with the correct name and extension: [model].[ext]. The model run folder can be found by selecting the folder icon button [⁽¹⁾], the flow model for a MODFLOW-6 model will be stored in the .\GWF subfolder, the model name will correspond to the name of your conceptual model, and the extension will be the **Ext** value for the package in question. For example, if you will to run the horizontal flow barrier package (HFB), and you are running a model where:
 - the Visual MODFLOW Flex project file is called SiteModel.amd,
 - the Conceptual Model is called Concept1,
 - the Grid is called NumericalGrid,
 - the Run is called Run 1, and
 - the Flow Engine is MODFLOW-6

then the HFB file must be saved as: .\SiteModel.data\MODFLOW\NumericalGrid\Run1\MODFLOW-6\GWF\Concept1.DRT

If the above conditions are met, the custom package file will inserted into the relevant .NAM file and run with the model. Note that certain results from unsupported packages will not be read back into Visual MODFLOW Flex, such as the flow balance terms associated with the SFR package.

Common Options

The following settings are available for the options block in many packages:

~ C	PTIONS	
В	OUNDNAMES	Yes
N	lover	No
P	RINT_FLOWS	No
P	RINT_INPUT	No
S	AVE_FLOWS	Yes
U	Jse as Obs Targets	No
U	Jse Time Series	No

• **Boundnames**: Yes/No switch to indicate whether or not boundnames will be used. If set to yes, then the name(s) of the boundary condition(s) of the given type will be added as boundnames to the package file and MODFLOW-6 will track flows and

volumes in the mass budget separately for these boundaries. The Boundnames option is set to yes by default.

- PRINT_FLOWS: Yes/No switch to indicate whether the list of flow rates through the given package type will be printed to the listing file for every stress period time step for which the Print to .LST > Budget is selected in the <u>Output Control</u> settings.The PRINT_FLOWS option is set to yes by default.
- SAVE_FLOWS: Yes/No switch to indicate whether cell-by-cell flow rates through the given package type will be written to the budget file for every stress period time step for which the Save to Binary > Budget is selected in the <u>Output Control</u> settings.The SAVE_FLOWS option is set to yes by default.

Additional options (e.g. Mover, Use as Obs Targets, Use Time Series) are included as readonly options. Support for these options will be added in future versions of Visual MODFLOW Flex. In the meantime, these options may be included in the simulation through manual edits to translated files. For more details please refer to the MODFLOW-6 Description of Input and Output manual (USGS, <u>2022</u>).

MODFLOW-6 - Flow Packages

Package-specific settings for MODFLOW-6 flow model packages are described below:

NPF Settings

The following settings are specific to the node property flow (NFP) package:

~	General				
	Ext	.NPF			
	Run	Yes			
	Translate	Yes			
~	GRIDDATA				
	ANGLE1	(Collection)			
	ANGLE2	(Collection)			
	ANGLE3	(Collection)			
~					
	ALTERNATIVE_CELL_AVERAGING	AMT_HMK			
	AnglesByCell	No			
	CellType	ByLayer			
	DEWATERED	No			
	PERCHED	No			
	SAVE_FLOWS	Yes			
	SAVE_SATURATION	No			
	SAVE_SPECIFIC_DISCHARGE	No			
	THICKSTRT	No			
	TVK6	No			
	VARIABLECV	No			
	WETDRY	Global			
	XT3D	None			

Options

- Alternative Cell Averaging This setting allows you to select how MODFLOW-6 will calculate intercell conductance:
 - AMT_HMK [Default]: is "arithmetic-mean thickness and harmonic-mean hydraulic conductivity" method of computing transmissivity
 - AMT_LMK: is "arithmetic-mean thickness and logarithmic-mean hydraulic conductivity" method of computing transmissivity (assumes the aquifer is flat with a water table in which hydraulic conductivity varies linearly between nodes);
 - Logarithmic: is "logarithmic-mean" method (assumes transmissivity varies linearly between nodes);
- **DEWATERED** If the *dewatered* option is set to yes, then the vertical conductance is calculated using only the saturated thickness and properties of the overlying cell if the head in the underlying cell is below its top. The *dewatered* option is off by default.
- **PERCHED** If the *perched* option is set to yes, when a cell is overlying a dewatered convertible cell (see option above), the head difference used in Darcy's Law is equal to the head in the overlying cell minus the bottom elevation of the overlying cell. If not specified, then the default is to use the head difference between the two cells. The *perched* option is off by default.
- SAVE_SATURATION If the SAVE_SATURATION option is set to yes, the cell saturation will be written as a term in the budget file, for every stress period time step for which the Save to Binary > Budget is selected in the <u>Output Control</u> settings. The SAVE_SATURATION option is set to no by default.

- SAVE_SPECIFIC_DISCHARGE If the SAVE_SPECIFIC_DISCHARGE option is set to yes, then MODFLOW-6 will calculate the x, y, and z components of specific discharge (at cell centers) and write the values to the budget file, for every stress period time step for which the Save to Binary > Budget is selected in the <u>Output</u> <u>Control</u> settings. The SAVE_SPECIFIC_DISCHARGE option is set to no by default. Note that Visual MODFLOW Flex calculates these terms for the velocity outputs so it is not required/redundant.
- THICKSTRT If the THICKSTRT option is set to yes, then cells having a negative ICELLTYPE are confined, and their cell thickness for conductance calculations will be computed as STRT-BOT rather than TOP-BOT. Note that Visual MODFLOW Flex currently only translates ICELLTYPE = 1. The THICKSTRT option is set to no by default.
- VARIABLE_CV If the VARIABLE_CV option is set to yes, then the vertical conductance will be calculated using the saturated thickness and properties of the overlying cell and the thickness and properties of the underlying cell. If the DEWATERED keyword is also set to yes, then the vertical conductance is calculated using only the saturated thickness and properties of the overlying cell if the head in the underlying cell is below its top. If both these options are set to no, then the default condition is to calculate the vertical conductance at the start of the simulation using the initial head and the cell properties. The vertical conductance remains constant for the entire simulation. The VARIABLE_CV is set to no by default.

Grid Data Block

The parameters described below can be specified on a per-layer basis using a collection. To access the desired collection, click in the (Collection) cell and then click the ... button. You can select more than one layer simultaneously using the mouse pointer and the [SHIFT] and [CTRL] keys and define the criteria simultaneously for the selected layer(s).

- **Angle1** is a rotation angle of the hydraulic conductivity tensor in degrees. The angle represents the first of three sequential rotations of the hydraulic conductivity ellipsoid. With the K11 (Kx), K22 (Ky), and K33 (Kz) axes of the ellipsoid initially aligned with the x, y, and z coordinate axes, respectively. ANGLE1 rotates the ellipsoid about its K33 axis (within the x y plane). A positive value represents counter-clockwise rotation when viewed from any point on the positive K33 axis, looking toward the center of the ellipsoid. A value of zero indicates that the K11 axis lies within the x z plane. If ANGLE1 is not specified, default values of zero are assigned to ANGLE1, ANGLE2, and ANGLE3, in which case the K11, K22, and K33 axes are aligned with the x, y, and z axes, respectively.
- **Angle2** is a rotation angle of the hydraulic conductivity tensor in degrees. The angle represents the second of three sequential rotations of the hydraulic conductivity ellipsoid. Following the rotation by ANGLE1 described above, ANGLE2 rotates the ellipsoid about its K22 axis (out of the x y plane). An array can be specified for ANGLE2 only if ANGLE1 is also specified. A positive value of ANGLE2 represents clockwise rotation when viewed from any point on the positive K22 axis, looking toward the center of the ellipsoid. A value of zero indicates that the K11 axis lies within the x y plane. If ANGLE2 is not specified, default values of zero are assigned to ANGLE2 and ANGLE3; connections that are not user-designated as vertical are assumed to be

strictly horizontal (that is, to have no z component to their orientation); and connection lengths are based on horizontal distances.

• **Angle3** - is a rotation angle of the hydraulic conductivity tensor in degrees. The angle represents the third of three sequential rotations of the hydraulic conductivity ellipsoid. Following the rotations by ANGLE1 and ANGLE2 described above, ANGLE3 rotates the ellipsoid about its K11 axis. An array can be specified for ANGLE3 only if ANGLE1 and ANGLE2 are also specified. An array must be specified for ANGLE3 if ANGLE2 is specified. A positive value of ANGLE3 represents clockwise rotation when viewed from any point on the positive K11 axis, looking toward the center of the ellipsoid. A value of zero indicates that the K22 axis lies within the x - y plane.

STO Settings

The following settings are specific to the storage (STO) package:

~	General		
	Ext	.STO	
	Run	Yes	
	Translate	Yes	
\mathbf{v}	OPTIONS		
	SAVE_FLOWS	Yes	
	SS_CONFINED_ONLY	No	
	TVS6	No	

The storage package is only translated if the Model Run Type is set to Transient in the MODFLOW Settings.

Options

SS_CONFINED_ONLY - If the SS_CONFINED_ONLY option is set to yes, then compressible storage is only calculated for a convertible cell (ICONVERT>0) when the cell is under confined conditions (head greater than or equal to the top of the cell). This option has no effect on cells that are marked as being always confined (ICONVERT= 0). This option is identical to the approach used to calculate storage changes under confined conditions in MODFLOW-2005. Note that Visual MODFLOW Flex currently only translates ICONVERT=1. The SS_CONFINED_ONLY option is set to no by default.

WEL Settings

The following settings are specific to the Well (WEL) package:

×	General		
	Ext	.WEL	
	Run	Yes	
	Translate	Yes	
~	OPTIONS		
	AUTO_FLOW_REDUCE	No	
	AUTO_FLOW_REDUCE_CSV	No	
	AUTO_FLOW_REDUCE_THRESHOLD	0.1	
	BOUNDNAMES	Yes	
	Mover	No	
	PRINT_FLOWS	No	
	PRINT_INPUT	No	
	SAVE_FLOWS	Yes	
	Use as Obs Targets	No	
	Use Time Series	No	

Options

- AUTO_FLOW_REDUCE If the AUTO_FLOW_REDUCE option is set to yes, then the AUTO_FLOW_REDUCE_THRESHOLD value (see below) will be read.By default, AUTO_FLOW_REDUCE is set to no and negative pumping rates are not reduced during a simulation.
- AUTO_FLOW_REDUCE_CSV If both this option and AUTO_FLOW_REDUCE are set to yes, then a new record will be written for each well in the well group for each time step in which the user-requested extraction rate is reduced by the program to a the : .\GWF\{Conceptual Model}.{Well Group}.WEL.csv. AUTO FLOW REDUCE CSV is set to no by default.
- AUTO_FLOW REDUCE_THRESHOLD a value used to define the fraction of the cell thickness used as an interval for smoothly adjusting negative pumping (i.e. withdrawal) rates to 0 in cells with head values less than or equal to the bottom of the cell. Negative pumping rates are adjusted to 0 or a smaller negative value when the head in the cell is equal to or less than the calculated interval above the cell bottom. AUTO_FLOW_REDUCE is set to 0.1 if the specified value is less than or equal to zero. By default, AUTO_FLOW_REDUCE is set to no and negative pumping rates are not reduced during a simulation.

EVT Settings

The following settings are specific to the Evapotranspiration (EVT) package:

~	General	
	Ext	.EVT
	Run	Yes
	Translate	Yes
~	OPTIONS	
	BOUNDNAMES	Yes
	FIXED_CELL	No
	FORMAT	AsArray
	PRINT_FLOWS	No
	PRINT_INPUT	No
	SAVE_FLOWS	Yes
	Use as Obs Targets	No
	Use Time Series	No

Options

- **FIXED_CELL** if this option is set to yes, then evapotranspiration will not be reassigned to a cell underlying the cell if that cell is inactive. If this option is set to no, then evapotranspiration will be applied to the uppermost active cell. This option is set to no by default.
- FORMAT there are two methods of inputting evapotranspiration data:
 - o AsArray [default] evapotranspiration data will be written to a layer-based array
 - AsList evapotranspiration data will be written to a list of cells along with the corresponding cell id

RCH Settings

The following settings are specific to the Recharge (RCH) package:

~	General	
	Ext	.RCH
	Run	Yes
	Translate	Yes
\mathbf{v}	OPTIONS	
	BOUNDNAMES	Yes
	FIXED_CELL	No
	FORMAT	AsArray
	PRINT_FLOWS	No
	PRINT_INPUT	No
	SAVE_FLOWS	Yes
	Use as Obs Targets	No
	Use Time Series	No

Options

• FIXED_CELL - if this option is set to yes, then recharge will not be reassigned to a cell underlying the cell if that cell is inactive. If this option is set to no, then recharge will be applied to the uppermost active cell. This option is set to no by default.

- FORMAT there are two methods of inputting recharge data:
 - o AsArray [default] recharge data will be written to a layer-based array
 - AsList recharge data will be written to a list of cells along with the corresponding cell id

OC Settings

The following settings are specific to the Output Control (OC) package:

~	General					
	Ext	.OC				
	Run	Yes				
	Translate	Yes				
\sim	OPTIONS					
	BUDGETCSV	No				
\sim	OPTIONS/PRINT_FORMAT					
	COLUMNS	1				
	DIGITS	4				
	FORMAT	General				
	WIDTH	20				

Options

• **BUDGET_CSV** - if this option is set to yes, then a CSV file containing the budget summary similar to what is printed in the list file will be created during the simulation. A budget summary will be printed for each time step in the simulation. This option is set to no by default.

Options/Print Format

The following options relate to the numerical format of the BUDGET_CSV file (if the option is set to yes):

- Columns: the number of columns for writing data
- Digits: the number of digits to use for writing a number
- Width: the number of characters that will be used to write numbers, including white space
- Format: the number format can be: General [default], Fixed, Exponential, or Scientific

DIS(V) Settings

The following settings are specific to the Discretization (by Vertices) (DIS/V) package:

~	General	
	Ext	.DIS
	Run	Yes
	Translate	Yes
\sim	OPTIONS	
	NOGRB	No

Options

• **NOGRB** - if this option is set to yes, then MODFLOW-6 will not create a binary grid file. The binary grid file is a common file format for the grid that is used by other modeling codes such as MOD-PATH3DU and certain PEST utilities. This option is set to no by default and a binary grid file will be created.

CHD Settings

The following settings are specific to the specified head (CHD) package:

~	General	
	Ext	.CHD
	Run	Yes
	Translate	Yes
~	OPTIONS	
	BOUNDNAMES	Yes
	PRINT_FLOWS	No
	PRINT_INPUT	No
	SAVE_FLOWS	Yes
	Use as Obs Targets	No
	Use Time Series	No
\mathbf{v}	Misc	
	Duplicate CHD6 Cell Filter	Average

- **Duplicate CHD Cell Filter** When working with conceptual models, in some cases multiple constant head cells may be assigned to the same cell. When MODFLOW formulates the system of equations, it simply adds boundary conditions for all other boundary conditions this is usually not a problem as these values still require a head solution for that cell; however adding the constant head values together typically does not produce the desired result. Therefore, Visual MODFLOW Flex includes an optional filter to handle these cases on translation:
 - *Minimum* the minimum specified head value for the current stress period in the cell(s) with multiple values will be assigned
 - Maximum the maximum specified head value for the current stress period in the cell(s) with multiple values will be assigned
 - Average [Default] the arithmetic mean of specified head values for the current stress period in the cell(s) with multiple values will be assigned
 - Sum specified head values values for the current stress period in the cell(s) with multiple values will be added.

SIM Settings

The following settings are specific to the specified head MODFLOW Simulation file (MFSIM.NAM):

\sim	General						
	Ext	.NAM					
	Run	Yes					
	Translate	Yes					
\sim	OPTIONS						
	CONTINUE	No					
	MAXERRORS	10					
	MEMORY_PRINT_OPTION	None					
	NOCHECK	No					

- **CONTINUE** if this option is set to yes, then MODFLOW-6 will continue with the remaining solution groups if one or more solutions do not converge. For example, if a transport model does not converge, then the flow model may continue through the rest of the simulation. By default, this option is set to no and the simulation will stop if any model in the simulation does not converge within the specified number of iterations.
- MAXERRORS maximum number of errors that will be stored and printed.
- **MEMORY_PRINT_OPTION** is a flag that controls printing of detailed memory manager usage to the end of the simulation list file.
 - o NONE [default] means do not print detailed information.
 - o SUMMARY means print only the total memory for each simulation component.
 - o ALL means print information for each variable stored in the memory manager.
- NOCHECK if this option is set to yes, then MODFLOW-6 will not perform checks on the model input files. Checks are performed by default.

NAM Settings

The following settings are specific to the Flow Model Name (NAM) file:

~	General	
	Ext	.NAM
	Run	Yes
	Translate	Yes
~	OPTIONS	
	NEWTON	Yes
	PRINT_FLOWS	Yes
	PRINT_INPUT	No
	SAVE_FLOWS	Yes
	UNDER_RELAXATION	Yes

- **NEWTON** if this option is set to yes, then the simulation will use the Newton-Raphson formulation for groundwater flows between connected, convertible groundwater cells and stress packages that support calculation of Newton-Raphson terms for groundwater exchanges. Cells will not dry when this option is used. By default, the Newton-Raphson formulation is applied.
- UNDER-RELAXATION if this option is set to yes, the groundwater head in a cell will be underrelaxed when water levels fall below the bottom of the model below any given cell. By default this option is set to yes, and the Newton-Raphson UNDER_RELAXATION is applied. This option is ignored if the NEWTON option is set to no.

11.8.3 MODFLOW-6 Transport

This chapter describes the features, functionality, and options in the Translation section of the Visual MODFLOW Flex interface when using MODFLOW-6 to perform the groundwater transport (GWT) simulation.



If you are not familiar with MODFLOW-6 and how it has been implemented in Visual MODFLOW Flex, it is <u>strongly</u> <u>recommended</u> that you familiarize yourself with the MODFLOW-6 framework and input file structure, particularly if you intend to use some of the advanced features available in MODFLOW-6 and/or you wish to work with the input files directly.

At a minimum, please read <u>Introduction to MODFLOW-6</u> and the subtopics in the present section.

MODFLOW-6 Groundwater Transport Model Settings:

- Settings MODFLOW-6 Transport
- Solver Settings
- Initial Concentrations
- Output Control
- Advanced Settings

11.8.3.1 MODFLOW-6 Transport Settings

The following general settings are available for the MODFLOW-6 transport engine:

Porosity Options

The Porosity options are used to select which porosity measurement to use for the transport solution.

- For advection-dominated transport, the best choice is to apply the "Effective" porosity option, then diffusion into and out of dead-end pore spaces can be considered negligible.
- For diffusion-dominated transport, the best choice is to select the "Total" porosity option to account for mass transfer to and from dead-end pore spaces.

11.8.3.2 Solver Settings

Solvers in MODFLOW-6 are handled through the iterative model solution (IMS) package which is used to solve flow and/or transport simulations. The IMS package uses a linear and non-linear methods to solve the simultaneous equations produced by the model(s) as described below:

tings Translation Log nam T	DIS	IMS	DIS	IC	OC	NPF	CHD	CHD(2)	RIV	WEL	STO	nam(2)
General	~	Gene										
Settings	Selected Solver Iterative Matrix Solver (IMS)									IS)		
MODFLOW-6												
Settings												
Solvers												
···· Initial Heads	~	Option	ns									
Output Control		PrintOption						Nor	e			
Advanced Settings		Comple						Sim				
MODFLOW-6 Transport-Specific		CsvOuterOutput			Fals							
General			erOutpu					Fals	e			
Solvers		NoPtc						First	-			
Initial Concentrations		AtsOut	erMaxim	umFract	ion			0.2	5			
Output Control	~	Linea	r									
i≟ Advanced Settings		InnerM	aximum					100				
		InnerD	VClose					1E-	06			
		InnerR	Close					1E-	06			
		Linear/	Accelera	tion				BIC	GStab			
		Relaxa	tionFact	or				0				
		Precon	ditionerl	evels				0				
		Precon	ditioner	Drop Tole	rance			0				
		Numbe	rOrthog	onalizatio	ons			0				
		Scaling	Method					Nor	e			
		Reorde	eringMet	hod				Nor	e			
	~	Nonlir										
			VClose					0.0	-			
			laximum					100				
			Relaxatio					Nor				
				nGamm	а			0.2				
			Relaxatio					0.7				
				nKappa				0.1				
				nMome	ntum			0.0	01			
			ackingN					10				
			-	olerance				10000				
			-	eduction				0.2				
		Backtr	ackingR	esidualL	imit			100				
	Pri	ntOptic	n									
								rom the sol				
		eans print nothing. SUMMARY means print only the total number of iterations and no sidual reduction summaries. ALL means print linear matrix solver convergence inform										
								convergen				

General Solution Options

The following settings are optional in the IMS package:

- **PrintOption**: An optional keyword setting that determines the print level of the solver in the listing file:
 - *Summary* means print only the total number of iterations and nonlinear residual reduction summaries.
 - All means print linear matrix solver convergence information to the solution listing file and model specific linear matrix solver convergence information to each model listing file in addition to Summary information.
 - None means that no solver information will be printed. This is the default option.
- **Complexity**: is an optional keyword that defines default non-linear and linear solver parameters.

- Simple indicates that default solver input values will be defined that work well for nearly linear models. This option is generally suitable for models that do not include nonlinear stress packages and models that are either confined or consist of a single unconfined layer that is thick enough to contain the water table within a single layer.
- Moderate: indicates that default solver input values will be defined that work well for moderately nonlinear models. This option is generally suited for models that include nonlinear stress packages and models that consist of one or more unconfined layers. The *Moderate* option should be used when the *Simple* option does not result in successful convergence.
- Complex: indicates that default solver input values will be defined that work well for highly nonlinear models. This option is generally suited for models that include nonlinear stress packages and models that consist of one or more unconfined layers representing complex geology and surface-water/groundwater interaction. The complex option should be used when the moderate option does not result in successful convergence.
- Custom: indicates that custom values will be defined for the linear and non-linear solvers.

If the Simple, Moderate, or Complex options are selected, then only the items in the linear and non-linear solver sections below marked with * will be translated. All other options will use the defaults below:

SETTINGS	COMPLEXITY							
SETTINGS	SIMPLE	MODERATE	COMPLEX					
NON-LINEAR SOLVER SE	TTINGS							
OUTER_DVCLOSE *	0.001	0.01	0.1					
OUTER_MAXIMUM *	25	50	100					
UNDER_RELAXATION	NONE	DBD	DBD					
UNDER_RELAXATION_TH ETA	1	0.9	0.8					
UNDER_RELAXATION_KA PPA	0	0.0001	0.0001					
UNDER_RELAXATION_G AMMA	0	0	0					
UNDER_RELAXATION_M OMENTUM	0	0	0					
BACKTRACKING_NUMBE R	0	0	20					
BACKTRACKING_TOLER ANCE	0	0	1.05					

BACKTRACKING_REDUC TION_FACTOR	0	0	0.1
BACKTRACKING_RESIDU AL_LIMIT	0	0	0.002
LINEAR SOLVER SETTINGS			
INNER_MAXIMUM *	50	100	500
INNER_DVCLOSE *	0.001	0.01	0.1
INNER_RCLOSE *	0.1	0.1	0.1
RCLOSE_OPTION	infinity-norm	infinity-norm	infinity-norm
LINEAR_ACCELERATION	CG	BICGSTAB	BICGSTAB
RELAXATION_FACTOR	0	0.97	0
PRECONDITIONER_LEVE LS	0	0	5
PRECONDITIONER_DRO P_TOLERANCE	0	0	0.0001
NUMBER_ORTHOGONALI ZATIONS	0	0	2
SCALING_METHOD	NONE	NONE	NONE
REORDERING_METHOD	NONE	NONE	NONE

- **CsvOuterOutput**: if this option is set to yes, then outer iteration convergence information will be written to a comma separated values file in the GWF subfolder. This option is off by default. Information written to this file includes maximum dependent-variable (for example, head or concentration) change convergence information at the end of each outer iteration for each time step.
- **CsvInnerOutput**: if this option is set to yes, then inner iteration convergence information will be written to a comma separated values file in the GWF subfolder. This option is off by default. Information written to this file includes maximum dependent-variable (for example, head or concentration) change and maximum residual convergence information for the solution and each model (if the solution includes more than one model) and linear acceleration information for each inner iteration.
- NoPTC: is a settings that is used to control the pseudo-transient continuation (PTC) options for steady state periods for models using the Newton-Raphson formulation (which is controlled by in NAM file <u>settings</u>):
 - o None: PTC will not be used in solution
 - o First. PTC will be activated for the first stress period
 - o All: PTC will be deactivated for all stress periods

For many problems, PTC can significantly improve convergence behavior for steadystate simulations, and for this reason it is active by default. In some cases; however, PTC can worsen the convergence behavior, especially when the initial conditions are similar to the solution. When the initial conditions are similar to (or exactly the same as) the solution and convergence is slow, then the NO_PTC FIRST option should be used to deactivate PTC for the first stress period. The NO_PTC ALL option should also be used in order to compare convergence behavior with other MODFLOW versions, as PTC is only available in MODFLOW 6.

• AtsOuterMaximumFraction: real value defining the fraction of the maximum allowable outer iterations used with the Adaptive Time Step (ATS) capability if it is active. If this value is set to zero by the user, then this solution will have no effect on ATS behavior. This value must be greater than or equal to zero and less than or equal to 0.5 or the program will terminate with an error. If it is not specified by the user, then it is assigned a default value of one third. When the number of outer iterations for this solution is less than the product of this value and the maximum allowable outer iterations, then ATS will increase the time step length by a factor of DTADJ in the ATS input file. When the number of outer iterations for this solution is greater than the maximum allowable outer iterations, then ATS (if active) will decrease the time step length by a factor of 1 / DTADJ.

Non-Linear Solver Options

The following settings are available for the Non-linear solver:

- OUTER_DVCLOSE: real value defining the dependent-variable (for example, head or concentration) change criterion for convergence of the outer (nonlinear) iterations, in units of the dependent-variable (for example, length for head or mass per length cubed for concentrations). When the maximum absolute value of the dependent-variable change at all nodes during an iteration is less than or equal to OUTER_DVCLOSE, iteration stops.
- **OUTER_MAXIMUM**: integer value defining the maximum number of outer (nonlinear) iterations. For a linear problem OUTER_MAXIMUM should be 1.
- UNDER_RELAXATION: an optional keyword that defines the nonlinear underrelaxation schemes used. Under-relaxation is also known as dampening, and is used to reduce the size of the calculated dependent variable before proceeding to the next outer iteration. Under-relaxation can be an effective tool for highly nonlinear models when there are large and often counteracting changes in the calculated dependent variable between successive outer iterations. By default under-relaxation is not used.
 - o NONE [Default] under-relaxation is not used
 - SIMPLE Simple under-relaxation scheme with a fixed relaxation factor (under relaxation gamma (see below)) is used.
 - o COOLEY Cooley under-relaxation scheme is used.
 - o DBD delta-bar-delta (DBD) under-relaxation is used.

Note that the under-relaxation schemes are often used in conjunction with problems that use the Newton-Raphson formulation (which is controlled by in NAM file <u>settings</u>); however, experience has indicated that they also work well for non-Newton problems, such as those with the wet/dry options of MODFLOW 6.

- UNDER_RELAXATION_GAMMA: a real value defining either the relaxation factor for the simple complexity scheme or the history or memory term factor of the Cooley and delta-bar-delta algorithms. For the simple scheme, a value of one indicates that there is no under-relaxation and the full head (or concentration) change is applied. This value can be gradually reduced from one as a way to improve convergence; for well behaved problems, using a value less than one can increase the number of outer iterations required for convergence and needlessly increase run times. Under relaxation gamma must be greater than zero for the simple scheme or the program will terminate with an error. For the Cooley and delta-bar-delta schemes, Under relaxation gamma is a memory term that can range between zero and one. When Under relaxation gamma is zero, only the most recent history (previous iteration value) is maintained. As Under relaxation gamma is increased, past history of iteration changes has greater influence on the memory term. The memory term is maintained as an exponential average of past changes. Retaining some past history can overcome granular behavior in the calculated function surface and therefore helps to overcome cyclic patterns of non-convergence. The value usually ranges from 0.1 to 0.3; a value of 0.2 works well for most problems. Under relaxation gamma is only used in the simulation if Under relaxation is not None.
- UNDER_RELAXATION_THETA: a real value defining the reduction factor for the learning rate (underrelaxation term) of the delta-bar-delta algorithm. The value of *under relaxation theta* is between zero and one. If the change in the dependent-variable (for example, head or concentration) is of opposite sign to that of the previous iteration, the under-relaxation term is reduced by a factor of *under relaxation theta*. The value usually ranges from 0.3 to 0.9; a value of 0.7 works well for most problems. *Under relaxation theta* is only used in the simulation if *under relaxation* is DBD.
- UNDER_RELAXATION_KAPPA: a real value defining the increment for the learning rate (under-relaxation term) of the delta-bar-delta algorithm. The value of *under relaxation kappa* is between zero and one. If the change in the dependent-variable (for example, head or concentration) is of the same sign to that of the previous iteration, the under-relaxation term is increased by an increment of *under relaxation kappa*. The value usually ranges from 0.03 to 0.3; a value of 0.1 works well for most problems. *Under relaxation kappa* is only used in the simulation if *under relaxation* is DBD.
- UNDER_RELAXATION_MOMENTUM: a real value defining the fraction of past history changes that is added as a momentum term to the step change for a nonlinear iteration. The value of *under relaxation momentum* is between zero and one. A large momentum term should only be used when small learning rates are expected. Small amounts of the momentum term help convergence. The value usually ranges from 0.0001 to 0.1; a value of 0.001 works well for most problems. *Under relaxation momentum* is only used in the simulation if *under relaxation* is DBD.
- **BACKTRACKING_NUMBER**: an integer value defining the maximum number of backtracking iterations allowed for residual reduction computations. If *backtracking*

number = 0 then the backtracking iterations are omitted. The value usually ranges from 2 to 20; a value of 10 works well for most problems.

- **BACKTRACKING_TOLERANCE**: a real value defining the tolerance for residual change that is allowed for residual reduction computations. The *backtracking tolerance* value should not be less than one to avoid getting stuck in local minima. A large value serves to check for extreme residual increases, while a low value serves to control step size more severely. The value usually ranges from 1.0 to 106; a value of 104 works well for most problems but lower values like 1.1 may be required for harder problems. *Backtracking tolerance* is only used in the simulation if *backtracking number* is greater than zero.
- **BACKTRACKING_REDUCTION_FACTOR**: real value defining the reduction in step size used for residual reduction computations. The value of is between zero and one. The value usually ranges from 0.1 to 0.3; a value of 0.2 works well for most problems. *Backtracking reduction factor* is only used in the simulation if *backtracking number* is greater than zero.
- **BACKTRACKING_RESIDUAL_LIMIT**: a real value defining the limit to which the residual is reduced with backtracking. If the residual is smaller than *backtracking residual limit*, then further backtracking is not performed. A value of 100 is suitable for large problems and residual reduction to smaller values may only slow down computations. *Backtracking residual limit* is used in the simulation if *backtracking number* is greater than zero.

Linear Solver Options

The following settings are available for the Linear solver:

- **INNER_MAXIMUM**: an integer value defining the maximum number of inner (linear) iterations. The number typically depends on the characteristics of the matrix solution scheme being used. For nonlinear problems, *inner maximum* usually ranges from 60 to 600; a value of 100 will be sufficient for most linear problems.
- INNER_DVCLOSE: a real value defining the dependent-variable (for example, head or concentration) change criterion for convergence of the inner (linear) iterations, in units of the dependent-variable (for example, length for head or mass per length cubed for concentration). When the maximum absolute value of the dependent-variable change at all nodes during an iteration is less than or equal to *inner dvclose*, the matrix solver assumes convergence. Commonly, *inner_dvclose* is set equal to or an order of magnitude less than the *outer_dvclose* value specified for the non-linear block.
- **INNER_RCLOSE**: a real value that defines the flow residual tolerance for convergence of the IMS linear solver and specific flow residual criteria used. This value represents the maximum allowable residual at any single node. Value is in units of length cubed per time, and must be consistent with MODFLOW-6 length and time units. Usually a value of 0.1 is sufficient for the flow-residual criteria when meters and seconds are the defined MODFLOW-6 length and time.

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- RCLOSE_OPTION: an optional keyword that defines the specific flow residual criterion used.
 - STR/CT: an optional keyword that is used to specify that *inner rclose* represents a infinity-Norm (absolute convergence criteria) and that the dependent-variable (for example, head or concentration) and flow convergence criteria must be met on the first inner iteration (this criteria is equivalent to the criteria used by the MODFLOW-2005 PCG package (Hill, <u>1990</u>)).
 - L2NORM_RCLOSE: an optional keyword that is used to specify that *inner rclose* represents a L-2 Norm closure criteria instead of a infinity-Norm (absolute convergence criteria). When *L2norm rclose* is specified, a reasonable initial *inner rclose* value is 0.1 times the number of active cells when meters and seconds are the defined MODFLOW-6 length and time.
 - RELATIVE_RCLOSE: an optional keyword that is used to specify that *inner rclose* represents a relative L-2 Norm reduction closure criteria instead of a infinity-Norm (absolute convergence criteria). When *relative rclose* is specified, a reasonable initial *inner rclose* value is 1.0×10⁻⁴ and convergence is achieved for a given inner (linear) iteration when *inner dvclose* and the current L-2 Norm is ≤ the product of the *relative_rclose* and the initial L-2 Norm for the current inner (linear) iteration. If *rclose option* is not specified, an absolute residual (infinity-norm) criterion is used.
 - LINEAR ACCELERATION: a keyword that defines the linear acceleration method used by the default IMS linear solvers.
 - o CG preconditioned conjugate gradient method.
 - o BICGSTAB preconditioned bi-conjugate gradient stabilized method.
 - **RELAXATION_FACTOR**: an optional real value that defines the relaxation factor used by the incomplete LU factorization preconditioners (MILU(0) and MILUT). *Relaxation_factor* is unitless and should be greater than or equal to 0.0 and less than or equal to 1.0. *Relaxation factor* values of about 1.0 are commonly used, and experience suggests that convergence can be optimized in some cases with relax values of 0.97. A *Relaxation factor* value of 0.0 will result in either ILU(0) or ILUT preconditioning (depending on the value specified for *preconditioner levels* and/or *preconditioner drop tolerance*). By default, *relaxation factor* is zero.
 - **PRECONDITIONER_LEVELS**: an optional integer value defining the level of fill for ILU decomposition used in the ILUT and MILUT preconditioners. Higher levels of fill provide more robustness but also require more memory. For optimal performance, it is suggested that a large level of fill be applied (7 or 8) with use of a drop tolerance. Specification of a *preconditioner levels* value greater than zero results in use of the ILUT preconditioner. By default, the number of *preconditioner levels* is zero and the zero-fill incomplete LU factorization preconditioners (ILU(0) and MILU(0)) are used.
 - PRECONDITIONER_DROP_TOLERANCE: a real value that defines the drop tolerance used to drop preconditioner terms based on the magnitude of matrix entries in the ILUT and MILUT preconditioners. A value of 10⁻⁴ works well for most problems. By default, the *preconditioner drop tolerance* is zero and the zero-fill incomplete LU factorization preconditioners (ILU(0) and MILU(0)) are used.

- NUMBER_ORTHOGONALIZATIONS: an integer value defining the interval used to explicitly recalculate the residual of the flow equation using the solver coefficient matrix, the latest dependent/variable (for example, head or concentration) estimates, and the right hand side. For problems that benefit from explicit recalculation of the residual, a number between 4 and 10 is appropriate. By default, the *number of orthogonalizations* is zero.
- SCALING_METHOD: an optional keyword that defines the matrix scaling approach used. By default, matrix scaling is not applied.
 - o NONE [Default] no matrix scaling applied.
 - DIAGONAL symmetric matrix scaling using the POLCG preconditioner scaling method in Hill (<u>1990</u>).
 - o L2NORM symmetric matrix scaling using the L-2 Norm.
- **REODERING_METHOD**: an optional keyword that defines the matrix reordering approach used. By default, matrix reordering is not applied.
 - o NONE [Default] original ordering.
 - o RCM reverse Cuthill McKee ordering.
 - *MD* minimum degree ordering.

11.8.3.3 Initial Concentrations

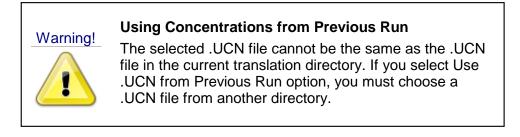
In Visual MODFLOW Flex, the Initial Concentrations are typically defined at the <u>Define</u> <u>Properties</u> step in the workflow. For more details, please see the section on setting <u>Initial</u> <u>Concentrations</u>. However, in some cases, it may be preferable to use alternate values from a previous model run. As such, the initial concentrations that will be translated for the simulation can be specified by species using the table shown below:

3 📀 🕨 Tanslate					
900					
Settings Translation Log nam TDIS IMS DIS	IC OC	NPF CHD CHD() RIV WEL STO nam(2)		
General	ld	Species Name	Option	FilePath	Browse
	001	Conc001	SPECIFIED		Browse
MOPLOW-S Transport-Specific General Solves Solves Solves Add Concentrations Odpa Control Advanced Settings					

- Id: The index of the species in the transport simulation as defined in the Modeling Objectives step.
- Species Name: The name of the species
- Option:
 - Specified [Default]: will use the values that are defined for "Initial Concentrations" at the Define Properties step.

 Previous_Run: requires you to select a .UCN file from a previous transport Run and specify the Time step to be used. The .UCN file must be based on the same grid type and number of cells in each applicable dimension (i.e. layer, row, and columns for a structured grid, and same number of layers and cells per layer for an unstructured grid).

Select previous UCN file		_		×
Time step			Brows	e
	Oł	<	Cance	el



11.8.3.4 Output Control

The Output Control options set the information and frequency of information written and saved to the MODFLOW-6 output files (see following figure).

 Define Modeling Objectives Define Properties Define Boundary Conditions 	Settings Translation Log							
Select Next Step	- General	🖋 Every Nth s	tep 1 🔳	Concentration	n (Print to 🗸 👻			
Define Observations	Settings				Save to bir	ary	Print to .L	ST
Define Particles	Settings	End Time	Stress Period	Time Step	Concentration	Budget	Concentration	Budget
🗄 🗹 Select Run Type	Solvers	0.13	1	1				
Single Run	Initial Heads	0.28	1	2				П
Translate	Output Control	0.44	1	3				
Run View Results	Advanced Settings	0.61	1	4			Π	
View Charts	MODFLOW-6 Transport-Specific General	0.81	1	5				
Wew Maps	Solvers	1.022	1	6	Π			
	Initial Concentrations	1.26	1	7				
	Output Control	1.51	1	8	Π			
	- Advanced Settings	1.8	1	9		Ē		
		2.11	1	10				
		2.45	1	11	Π	Π	Π	
		2.83	1	12				
		3.25	1	13	Π	Π	Π	Π
		3.71	1	14				
		4.21	1	15	Π	Π	Π	Π
		4.76	1	16				
		5.37	1	17				
		6.039	1	18				
		6.78	1	19				
		7.59	1	20				
		8.48	1	21				
		9.46	1	22				
		10.53	1	23				
		11.72	1	24				
		13.025	1	25				

By default, each MODFLOW-6 groundwater transport model simulation will produce several output files as described below. The Output Control settings allow you to specify the stress period(s)/time step(s) for which model results of interest will be written to these output files. The Output Control Settings are provided in a tabular format:

- Schedule:
 - End Time: the elapsed simulation time corresponding to the end of the specified stress period and time step
 - o Stress Period: the stress period in the schedule
 - o Time Step: the time step within the stress period
- Save to Binary:
 - Concentration: simulated heads will be written to the binary heads file (. \GWF\modelname.HDS) for active cells in the grid for selected End Times (Stress Period/Time Step)
 - Budget: mass budget terms will be written to the binary budget file (. \GWF\modelname.BGT) for active cells and boundary conditions in the grid for selected End Times (Stress Period/Time Step).

Please Note: for cell-by-cell values to be added to the budget file, the SAVE_FLOWS option must be enabled (set to "Yes") in the Advanced Settings for the NAM package. Similarly, for cell-to-boundary condition values to be added to the budget file, the SAVE_FLOWS option must be enabled in the Advanced Settings for each desired boundary condition (e.g. the SSM, CNC, and SRC packages). In Visual MODFLOW Flex, the SAVE_FLOWS option is enabled by default for all supported packages including the NAM file and supported boundary conditions.

 Print to LST: information will be written to the listing file (. \GWT\S###\modelname.LST), where S### is the index of each species:

- Concentration: simulated concentrations will be written to the listing file for active cells in the grid for selected End Times (Stress Period/Time Step). Note that this option should be used sparingly, typically for model troubleshooting, particularly as this format can lead to overly large output files that are less efficient to work with than the binary file or related files that can be exported from Visual MODFLOW Flex.
- Budget: net flow budget terms, expressed at a package level, for boundary conditions and internal storage will be written to the listing file for selected End Times (Stress Period/Time Step)

Please Note: for cell-by-cell values to be added to the listing file, the PRINT_FLOWS option must be enabled (set to "Yes") in the Advanced Settings for the NAM package. Similarly, for cell-to-boundary condition values to be added to the budget file, the PRINT_FLOWS option must be enabled in the Advanced Settings for each desired boundary condition. In Visual MODFLOW Flex, the PRINT_FLOWS option is enabled by default for all supported packages including the NAM file and supported boundary conditions.

Saving Output Every Nth Time Step

For simulations with many stress periods and time steps, it can be very tedious to manually select the desired output time step intervals. The row of fields underneath the Output Control table are used to specify regular time step intervals for saving files during Each N-th step in each stress period. The first text box is where the N value is entered. To apply this value to the column, click the underlying checkbox.

If a subsequent engine is included in the run formation (e.g. ZoneBudget) with the MODFLOW simulation, Visual MODFLOW Flex will save the flow terms for all time steps by default.

11.8.3.5 Advanced Settings

Advanced translation settings are available for transport simulations to enable more advanced control of translation and package settings. <u>General</u> and <u>common</u> settings are described in the section on the advanced settings for MODFLOW-6 groundwater flow (GWF) models, while package-specific settings are described below.

MODFLOW-6 - Transport Packages

Package-specific settings for MODFLOW-6 flow model packages are described below:

ADV Settings

The following settings are specific to the Advection (ADV) package:

✓ General		
Ext	.ADV	
Run	Yes	
Scheme	Upstream	
Translate	Yes	

- Scheme This setting allows you to select the solution technique for the transport:
 - o Upstream [Default]: upstream finite difference
 - o Central: central finite difference
 - o TVD: Higher-order Total Variation Diminishing method

These methods are described in more detail, here and here.

CNC Settings

The following settings are specific to the Constant Concentration (CNC) package:

\mathbf{v}	General	
	Ext	.CNC
	Run	Yes
	Translate	Yes
\mathbf{v}	OPTIONS	
	BOUNDNAMES	Yes
	PRINT_FLOWS	No
	PRINT_INPUT	No
	SAVE_FLOWS	Yes
	Use Time Series	No
\mathbf{v}	Misc	
	Duplicate CNC6 Cell Filter	Average

- **Duplicate CNC6 Cell Filter** When working with conceptual models, in some cases multiple constant concentration cells may be assigned to the same cell. When MODFLOW formulates the system of equations, it simply adds boundary conditions for all other boundary conditions this is usually not a problem as these values still require a concentration solution for that cell; however adding the constant concentration values together typically does not produce the desired result. Therefore, Visual MODFLOW Flex includes an optional filter to handle these cases on translation:
 - *Minimum* the minimum specified concentration value for the current stress period in the cell(s) with multiple values will be assigned
 - Maximum the maximum specified concentration value for the current stress period in the cell(s) with multiple values will be assigned
 - Average [Default] the arithmetic mean of specified concentration values for the current stress period in the cell(s) with multiple values will be assigned
 - Sum specified concentration values values for the current stress period in the cell(s) with multiple values will be added.

DSP Settings

The following settings are specific to the Dispersion (DSP) package and control how the <u>Dispersion</u> properties in the Define Properties workflow step will be translated:

\mathbf{v}	General	
	Ext	.DSP
	Run	Yes
	Translate	Yes
\mathbf{v}	OPTIONS	
	ALH - Longitudinal dispersivity in horizontal direction	No
	ALV - Longitudinal dispersivity in vertical direction	No
	ATH1 - Transverse dispersivity in horizontal direction	No
	ATH2 - Transverse dispersivity in horizontal direction	No
	ATV - Transverse dispersivity when flow is in vertical direction	No
	Mechanical Dispersion	No
	Molecular Diffusion	No
	XT3D	None

- ALH: a <u>read-only</u> setting for translating longitudinal dispersivity in the horizontal direction. If flow is strictly horizontal, then this is the longitudinal dispersivity that will be used. If flow is not strictly horizontal or strictly vertical, then the longitudinal dispersivity is a function of both ALH and ALV. If mechanical dispersion is included in the simulation (i.e. the Mechanical Dispersion setting is set to yes) then this settings is set to yes, otherwise, it is set to no.
- ALV: a setting for translating longitudinal dispersivity in the vertical direction. If flow is strictly vertical, then this is the longitudinal dispersivity that will be used. If flow is not strictly vertical, then the longitudinal dispersivity is a function of both ALH and ALV. If this option is set to no and mechanical dispersion is represented, then the ALV values in the dispersion array is not translated and assumed to equal ALH by MODFLOW-6.
- ATH1: a <u>read-only</u> setting for translating the transverse dispersivity in horizontal direction. This is the transverse dispersivity value for the second ellipsoid axis. If flow is strictly horizontal and directed in the x direction (along a row for a regular grid), then this value controls spreading in the y-direction. If mechanical dispersion is included in the simulation (i.e. the Mechanical Dispersion setting is set to yes) then this settings is set to yes, otherwise, it is set to no.
- ATH2: a setting for translating the transverse dispersivity in horizontal direction. This is the transverse dispersivity value for the third ellipsoid axis. If flow is strictly horizontal and directed in the x direction (along a row for a regular grid), then this value controls spreading in the z-direction. If this option is set to no and mechanical dispersion is represented, then this array is not translated and assumed to equal ATH1 by MODFLOW-6.
- **ATV**: a setting for translating the transverse dispersivity when flow is in vertical direction. If flow is strictly vertical and directed in the z-direction, then this value controls spreading in the x and y directions. If this option is set to no and mechanical dispersion is represented, then this array is not translated and assumed to equal ATH2 (or ATH1) by MODFLOW-6.

- **Mechanical Dispersion**: a setting for translating the dispersivity terms (ALH, ALV, ATH1, ATH2, ATV). If set to yes, then ALH and ATH1 will values will be translated and the other dispersivity terms (ALV, ATH2, and ATV) will be translated based on their settings; otherwise, none of these terms will be included and mechanical dispersion terms will be omitted from the solution.
- **Molecular Diffusion**: a setting for translating the diffusion term. If set to yes, then the molecular diffusion term will be included in the simulation.
- **XT3D**: a setting for (de)activating the XT3D method and has the following options:
 - None [Default]: the XT3D formulation will not be used in the solution. This method is generally faster and less accurate. This option may provide a fast and accurate solution under some circumstances, such as when flow aligns with the model grid, there is no mechanical dispersion, or when the longitudinal and transverse dispersivities are equal. This option may also be used to assess the computational demand of the XT3D approach by noting the run time differences with and without this option on.
 - *RHS*: the XT3D formulation will only add dispersion terms to the right-hand side terms in the system of equations for the transport solution. This option uses less memory, but may require more iterations than the full XT3D formulation available by using the Coefficients option.
 - Coefficients: the full XT3D formulation will used and dispersion terms will be added to the coefficient matrix in the system of equations for the transport solution. This option uses the most memory and may be computationally expensive; however, this option may be required to accurately represent dispersion.

FMI Settings

The following settings are specific to the Flow Model Interface (FMI) package and control whether and how the Groundwater Flow (GWF) and Groundwater Transport (GWT) models will be linked:

~	General	
	Ext	.FMI
	Run	Yes
	Translate	Yes
~	OPTIONS	
	Exchange	Linked
	Flow Imbalance Correction	No
	Save Flows	No

- Exchange: TBD
- Flow Imbalance Correction: TBD
- Save Flows: TBD

Please Note: the FMI package and GWT6 (Exchange) package are mutually exclusive.

IMST Settings

The following settings are specific to the Iterative Model Solution (IMS) package for Transport models (IMST):

~	General	
	Ext	.IMST
	Run	Yes
	Translate	Yes
	UseSpeciesSpecificClosures	No
~	Species	
	ClosureCriteria	(Collection)

- UseSpeciesSpecificClosures: is a setting that controls whether or not the Species-Specific ClosureCriteria (see below) will be used. This option is set to no by default.
- ClosureCriteria: Is a collection of species-specific settings that allows you to set independent solver <u>closure criteria</u> (i.e. INNER_DVCLOSE, INNER_RCLOSE, OUTER_DVCLOSE) for each species. This may be useful if the concentrations of the species are expected to vary over several orders of magnitude. To access the desired collection, click in the (Collection) cell and then click the ... button. You can select more than one layer simultaneously using the mouse pointer and the [SHIFT] and [CTRL] keys and define the criteria simultaneously for the selected layer(s).

IMSSpeciesType Collection Editor			?	\times
Members: 0 PCE 1 TCE 2 DCE 3 VC 4 ETH 5 CI-	↑ ↓	PCE properties: Misc INNER_DVCLOSE INNER_RCLOSE OUTER_DVCLOSE Species	1E-06 1E-06 0.01 001	
Add Remove		ОК	Cance	

IST Settings

The settings described below are specific to the Immobile Storage and Transfer (IST) package and will only be used if the <u>Transport Modeling Objectives</u> include either, the Dual Domain With Complex Sorption, the Triple Domain with Complex Sorption, or the Quadruple Domain with Complex Sorption Retardation Models.

Ext	.IST	
Run	Yes	
Translate	Yes	
OPTIONS		
BUDGET FILEOUT	conceptual-model.bgt	
BUDGETCSV FILEOUT	conceptual-model.bgt.csv	
CIM FILEOUT	conceptual-model.cim.ucn	
SAVE_FLOWS	Yes	
Species		
Immobile1	(Collection)	
Immobile2	(Collection)	
Immobile3	(Collection)	
	Run Translate OPTIONS BUDGET FILEOUT BUDGETCSV FILEOUT CIM FILEOUT SAVE_FLOWS Species Immobile1 Immobile2	Run Yes Translate Yes OPTIONS BUDGET FILEOUT conceptual-model.bgt BUDGETCSV FILEOUT conceptual-model.bgt.csv CIM FILEOUT conceptual-model.cim.ucn SAVE_FLOWS Yes Species Immobile1 (Collection) Immobile2 (Collection)

The following settings are available for the active immobile domain(s) in the Immobile Storage and Transfer package:

- Immobile1: is a collection of settings for the first immobile domain
- Immobile2: is a collection of settings for the second immobile domain
- Immobile3: is a collection of settings for the third immobile domain

Each one of these collections of settings can be accessed by clicking in the desired (Collection) cell and clicking the ... button, which will open the IST Immobile Domain Settings window with the following settings described below. You can select more than one layer simultaneously using the mouse pointer and the [SHIFT] and [CTRL] keys and define the criteria simultaneously for the selected layer(s).

DomainTypeWrapper Collection Edit	or			?	×
Members:	† *	 Select <u>P</u> ropertie		ticReacti tion	ions
Add <u>R</u> emove					
			ОК	Cance	el:

- **IREACT**: an option to specify the reaction model for the selected species in the selected immobile domain
 - NoKinetic Reaction: No kinetic reactions will be included in the simulation for the selected species
 - FirstOrderIrreversibleDecay: the selected species will be simulated for the selected species
 - *ZerothOrderIrreversibleDecay*: the selected species will be simulated for the selected species
- **ISOTHM**: an option to specify the retardation model for the selected species in the selected immobile domain
 - NoSorption: No sorption reactions will be included in the simulation for the selected species
 - o Linear: the linear sorption isotherm will be simulated for the selected species

MST Settings

The settings described below are specific to the Mobile Storage and Transfer (MST) package and will only be used if the <u>Transport Modeling Objectives</u> include either, the Dual Domain With Complex Sorption, the Triple Domain with Complex Sorption, or the Quadruple Domain with Complex Sorption Retardation Models.

~	General	
	Ext	.MST
	Run	Yes
	Translate	Yes
~	OPTIONS	
	SAVE_FLOWS	Yes
\mathbf{v}	Species	
	Mobile	(Collection)

The following settings are available for the active immobile domain(s) in the Immobile Storage and Transfer package:

• **Mobile**: is a collection of settings for the mobile domain. The mobile collection of settings can be accessed by clicking in the (Collection) cell and clicking the ... button, which will open the MST Mobile Domain Settings window with the following settings described below. You can select more than one species simultaneously using the mouse pointer and the [SHIFT] and [CTRL] keys and define the criteria simultaneously for the selected species(s).

DomainTypeWrapper Collection Edito	or			?	×
Members: 0 PCE 1 TCE 2 DCE 3 VC 4 ETH 5 CI-		Multi-Select Properties	: No Kinetic No Sorptic		DNS
<u>A</u> dd <u>R</u> emove		C	Ж	Cance	4

- **IREACT**: an option to specify the reaction model for the selected species in the selected immobile domain
- NoKinetic Reaction: No kinetic reactions will be included in the simulation for the selected species
- *FirstOrderIrreversibleDecay*: the selected species will be simulated for the selected species

- *ZerothOrderIrreversibleDecay*: the selected species will be simulated for the selected species
 - **ISOTHM**: an option to specify the retardation model for the selected species in the selected immobile domain
- NoSorption: No sorption reactions will be included in the simulation for the selected species
- o Linear: the linear sorption isotherm will be simulated for the selected species
- o Freundlich: the Freundlich isotherm will be simulated for the selected species
- o Langmuir: the Langmuir isotherm will be simulated for the selected species

OCT Settings

The following settings are specific to the Output Control for Transport (OCT) package:

~	General	
	Ext	.OCT
	Run	Yes
	Translate	Yes
~	OPTIONS	
	BUDGETCSV	No
~	OPTIONS/PRINT_FORMAT	
	COLUMNS	1
	DIGITS	4
	FORMAT	General
	WIDTH	20

Options

• **BUDGET_CSV** - if this option is set to yes, then a CSV file containing the budget summary similar to what is printed in the list file will be created during the simulation. A budget summary will be printed for each time step in the simulation. This option is set to no by default.

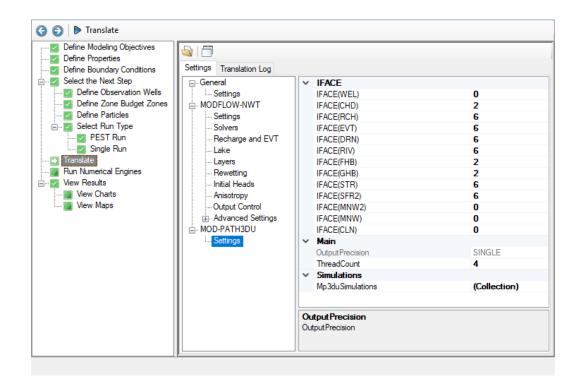
Options/Print Format

The following options relate to the numerical format of the BUDGET_CSV file (if the option is set to yes):

- Columns: the number of columns for writing data
- Digits: the number of digits to use for writing a number
- Width: the number of characters that will be used to write numbers, including white space
- Format: the number format can be: General [default], Fixed, Exponential, or Scientific

11.8.4 MOD-PATH3DU

The mod-PATH3DU program is used for calculating the advective flow pathlines and travel times for forward tracking and backward tracking particles for both finite difference and unstructured grids.



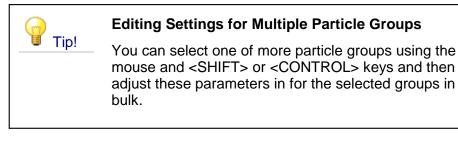
mod-PATH3DU has run-time settings for:

- IFACE: settings to assign boundary condition fluxes to cell faces:
 - o [0] Internal sink/source;
 - [2] Implicit side-face; flow is not explicitly assigned to a cell face, rather mod-PATH3DU distributes the flow to any side faces with zero flow;
 - \circ [5] Same as MODPATH. Flow through the bottom face of a cell;
 - o [6] Same as MODPATH. Flow through the top face of a cell;
 - \circ [7] Internal sink/source. Flow is assigned to the top face.
- ThreadCount: The number of Threads to use for processing particle tracks
- Mp3duSimulations: Opens a dialog for assigning settings for individual particle groups:

Mp3duSimulation Collection Editor				?	×
Members:	Riv	ers properties:			
0 Rivers 1 Wells		2↓ □			
+	~	General ADAPTIVE_STEP_ERROR	1E-06		
		CAPTURE_RADIUS	1		
		DIRECTION	BACKWARD		
		EULER_DT	0.01		
		GROUP_ID	0000000-0000-0000-0000	00000000)
		INITIAL_STEPSIZE	0.1		
		MAX_STEPSIZE	1000000		_
		NAME	Rivers		_
		SIMULATION_END_TIME	100000000000		
		STAGNATION_DT	0.01		_
	~	Options			
		DISPERSION RETARDATION	False False		
		RUN	True		
		TRACK_TO_TERMINATION	True		
		Three_ro_renmin/thom	1100		
Add Remove					
			ОК	Cancel	

Each particle group (shown on the left side of the dialog) has the following set of parameters (shown on the right) specified:

- Adaptive Step Error: The error criterion used to determine the maximum allowed error in all directions for the adaptive step size procedure.
- **Capture Radius**: the radial distance from within which a particle will be considered captured by a pumping well.
- **Direction**: this parameter is set when creating/editing the particle group and is disabled.
- **Euler DT**: the step size below which the Euler method is used instead of the Runge-Kutta method.
- Initial Step Size: The initial particle tracking stepsize
- Max Step Size: The maximum particle tracking stepsize
- Name: The name of the particle group
- **Simulation End Time**: Can be used to overwrite the simulation end time in the model. The default value is the flow model end time for forward simulations and 0 for backward simulation
- Stagnation DT: The tracking size below which a particle is considered stagnated.
- Run: Whether or not Flex will translate and run the particle group
- **Track To Termination**: Track the particles in the group on the last time step until each particle terminates at a boundary or is removed by reaching a stagnation point.



Please refer to the mod-PATH3DU <u>documentation</u> for more information about the settings listed above.

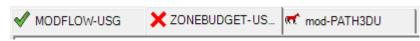
11.9 Run Engines

At this step, you can run the set of engines selected at the Single Run step.

The Run button will run the selected numeric engines using the required data files already present in the project folder the were generated at the <u>Translation</u> Step. If the required files are not present in the project folder, the numeric engines will not run. A warning message will appear indicating that the Visual MODFLOW files will not be translated prior to running the model.

Starting a Model Run

At the Run Numerical Engines Step, separate tabs will be generated for each engine or postprocessing utility selected at the single run step. The particle tracking utilities may generate multiple tabs depending on the number and type of particle groups to be simulated:



Press the **P**^{Run} button to start the simulation. The models will run in succession:

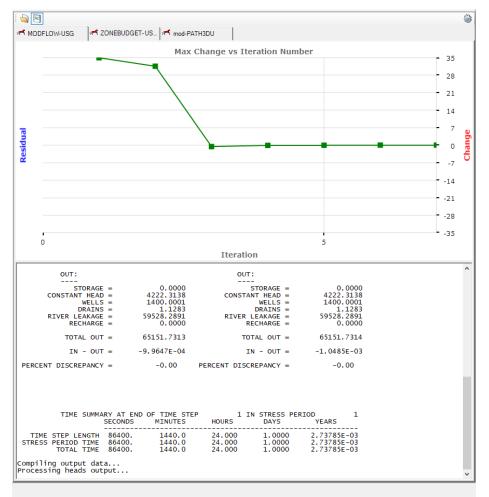
- Engines waiting to be run will be denoted by a static horse icon
- The currently active engine or utility will be denoted by a running horse icon
- Engines that have successfully completed will be denoted by a green checkmark
- Engines that failed to run or ran with errors will be denoted by a red "x"

Model Run Progress

During a flow and/or transport engine run, Visual MODFLOW Flex will provide feedback on the progression of the model run in a text console. By default, Visual MODFLOW Flex will also display an optional chart with the solution progress by iteration reported by the engine's solver, including:

• the maximum change in the heads relative to the previous iteration

At this step, run the MODFLOW engine. During a run you will see the Stress Period and Time Step count. Upon a successful run, you will see a budget summary from the .LST file:



Note that MODFLOW-6 models will show one chart for each model included in the solution (e.g. a groundwater flow model (GWF) solution and one groundwater transport model (GWT) solution for each species)

Chart Controls

The chart can be toggled on and off by clicking the plot button (\geq). You can also change the display settings the chart by clicking the Run View Settings button (\circledast):

🔜 Run View Settings	\times
Iterations to Display All Specified 300	
Dynamic Rescaling Enable Data Zoom Reduce scale after 50 () iterations have values that are less than half the current scale.	
OK Cancel	

Iterations to Display - allows you to select how many iterations to show. If a specified number is selected, then only that many of the most recent iterations will be displayed

Dynamic Rescaling - allows you to select whether the vertical axes of the chart will be rescaled after a given number of iterations

Model Run Completion

When the run completes additional information including the run time and other diagnostics will be to the text console of each engine. Model output will also be added to Run > Output folder in the Model Explorer:

Flow Engine Outputs

The following nodes will be added to the Output folder on the Model Explorer:

- Heads,
- Drawdown,
- Flooded Cells,
- Budget,
- · Velocity, and
- Water Table

Transport Engine Outputs

One node will be added per simulated species for simulations including groundwater transport using MODFLOW-6. A separate node for each species will also be added sorbed concentrations and for each immobile domain, if included included in the Modeling

Objectives. One or more residuals nodes may be added if concentration observations were added to the run.

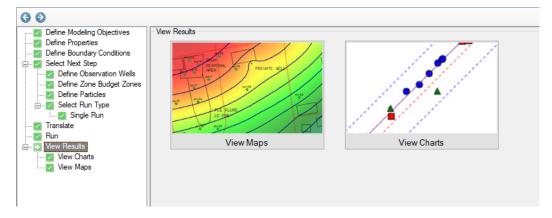
Particle Tracking Outputs

One node will be added per particle group with pathline information, if particle tracking was included as part of the simulation.

When you have finished reviewing the model run results, click 🕏 (Next Step) button to proceed to the View Results step.

11.10 View Results

At the View Results step, you have the option to <u>View Maps</u> or <u>View Charts</u>.



View Maps

At the <u>View Maps</u> step, you can visualize many different types of model outputs:

- Heads, drawdown, budget, velocity water table, flooded cells;
- Residuals (if observations were included in the simulation); and
- Pathlines (if particle tracking was included in the simulation).

View Charts

At the <u>View Charts</u> step, you can visualize results in a variety of chart types:

- <u>Calibration Dashboard</u>
 - o Observed vs. Calculated Heads
 - o Time Series
- Zone Budget

11.10.1 View Maps

The options for interpreting results from a MODFLOW-USG run are very similar to the <u>options</u> those from a finite difference (e.g. MODFLOW-2005) run. The section below describes the options and settings that specific to working with unstructured grids:

Following a successful model simulation, outputs are generated and Outputs branch in the Model Explorer tree for the active run.

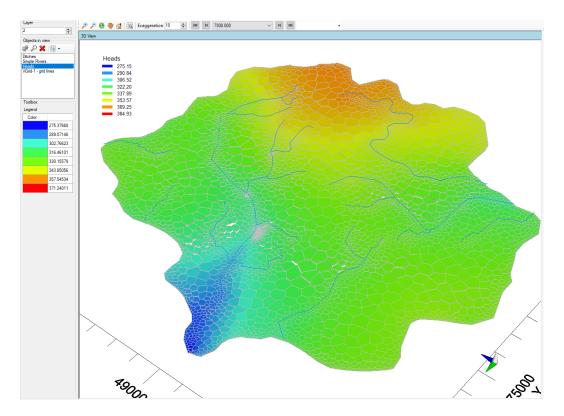
- Flow Engine Outputs
 - o Heads and Drawdown
 - o <u>Budget</u>
 - o <u>Velocity</u>
 - o Water Table
 - o Flooded Cells
 - o Residuals
- Pathlines

Flow Engine Outputs

Upon successful completion of a flow engine simulation, heads and related outputs can be visualized at the View Maps step as discussed below.

Heads and Drawdown

At the View Maps step, you can view contours and color shading of the flow engine results.



By default, you will see color shading and contours of the calculated heads for a layer slice of the model. You can also display heads along a row or column slice (based on a percent across the model domain in the X- and Y-directions, respectively) or using any of the other 3D Gridded Data Settings, as described in USG: View and Edit Properties.

If your model is transient, use the time controls above the 3D Viewer to change the output time; as you do this, the viewer will refresh to show the heads for the new output time.

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The display settings (color classes, contour line intervals, etc.) for the Heads can be adjusted in the Style settings. To load these settings, right click on Heads or Drawdown in the Outputs section of the Model Explorer, and select "Settings". For more details about these settings, see the section on <u>3D Gridded Data Settings</u>.

The exact same settings are available for viewing Drawdown results.

Budget

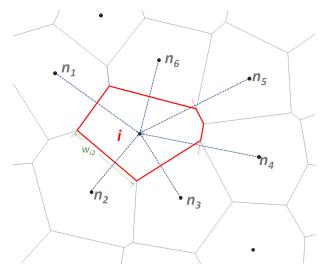
At the View Maps step, you can view cell-by-cell flows (read from the MODFLOW .BGT file). Once displayed in the viewer, load the Style settings for Budget, and choose the desired display type (Cells is turned on by default). Under the Colors panel (shown below), you can select from various Budget attributes:

- XRate: lateral flow into the cell along the direction of the X-axis
- YRate: lateral flow into the cell along the direction of the Y-axis

- **ZRate:** vertical flow into the cell from cells in the upper and lower layer face (adjacent layers)
- InFlowRate: total flow into the cell from all adjacent cells
- OutFlowRate: total flow out of the cell from all adjacent cells
- NetFlowRate: InFlowRate OutFlowRate
- One term will be also added for each active boundary condition type with external flows in the model simulation (e.g. Wells, Drains, Recharge, Constant Heads, Rivers, etc.).

Calculation Cell Flow-in/ Flow-out Based on Inter-Cell Flow Terms

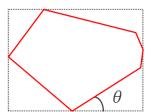
Inter–cell flow terms are saved in the output budget/cell-by-cell file (.CBC) for the neighbors of a given cell(i) and resolved to component flows in the principal directions (X, Y, and Z). For a given unstructured cell, there are an arbitrary number of faces in the horizontal plane, plus neighboring cells above and below (although a cell in the top layer will not have a neighboring cell above and a cell in the bottom layer will not have a neighboring cell below). For example in the cell below: there are six lateral neighbors (plus one above and one below).



Indices for the six adjacent cell faces $(n_1 - n_6)$ surrounding cell i.

The component flows for the faces are given by:

$$XRate = Q_{ix} = \sum_{\substack{j=1\\ n}}^{n} \frac{-Q_{ij}}{\sin\theta}$$
$$YRate = Q_{iy} = \sum_{\substack{j=1\\ j=1}}^{n} \frac{-Q_{ij}}{\cos\theta}$$



$$ZRate = Q_{iz} = \sum_{j=1}^{n} - Q_{ik}$$

where:

 Q_{ix} is the net flow in the ith cell in the X-direction

 Q_{iy} is the net flow in the ith cell in the Y-direction

 Q_{iz} is the net flow in the ith cell in the Z-direction

 Q_{ij} is the lateral flow between the ith cell and the jth neighboring cell

 $\boldsymbol{\theta}$ is the counterclockwise angle between the X-axis and the shared face between cells i and j

 Q_{ik} is the vertical flow between the ith cell and the kth neighboring cell above/below

InFlowRate (Flow In): total amount of flow into that cell is calculated by summing all positive flows into the cell from neighbors.

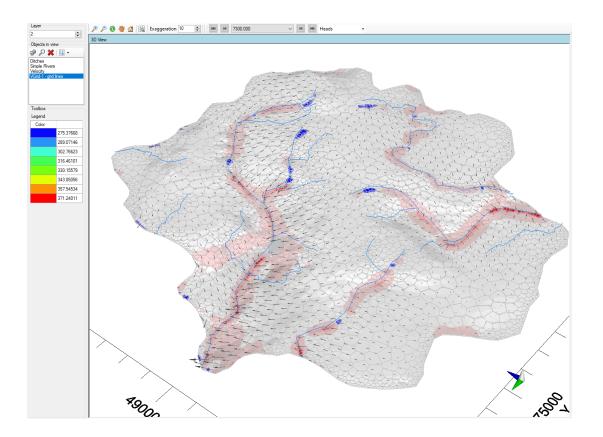
OutFlowRate (Flow Out): total amount of flow out of that cell is calculated by summing all negative flows out of the cell from neighbors.

NetFlowRate: the net amount of flow in/out of that cell is calculated by summing all flows in/out of the cell from neighbors

The Budget also includes one term for the net flow in/out of the cell via each boundary condition type active in the model.

Velocity

At the View Maps step, you can view groundwater velocities in a variety of ways as described in the section on <u>3D Gridded Data Settings</u>. By default, velocities are shown as <u>vectors</u>.



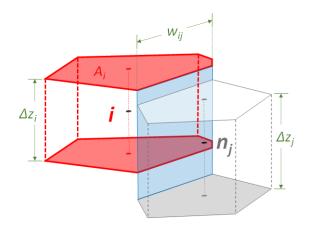
Calculation of Velocities in Visual MODFLOW Flex for Unstructured Grids

Model velocities are estimated in Visual MODFLOW Flex using a two-step process:

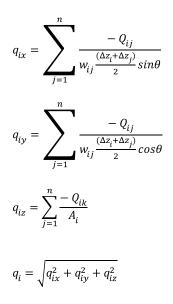
- 1. Estimate inter-cell velocities at each cell face in each component direction (X, Y, and Z)
- 2. Interpolate component velocities to the cell centroid

Inter-cell Darcy Velocity and Average Linear Velocity

Inter-cell fluxes (also know as Darcy velocities) are calculated in Visual MODFLOW Flex using a similar approach as the calculation for flows discussed above. The difference is that the flux calculation includes the area of the faces between shared cells. For neighboring cells, this area is the shared width and the average thickness of the cell and its neighbor.



Shared face and flux between a cell (i) and its neighbor (n_i) .



where:

 q_{ix} is the net flux/Darcy velocity in the ith cell in the X-direction

 q_{iy} is the net flux/Darcy velocity in the ith cell in the Y-direction

 q_{iz} is the net flux/Darcy velocity in the ith cell in the Z-direction

 ${}^{\it W}\!{}_{ij}$ is the width of the shared facet edge between the $i^{\rm th}$ cell and the $j^{\rm th}$ neighboring cell

 Δz_i is the thickness of the ith cell

 Δz_j is the thickness of the jth neighboring cell

 $\boldsymbol{\theta}$ is the counterclockwise angle between the X-axis and the shared face between cells i and j

 Q_{ik} is the vertical flow between the ith cell and the kth neighboring cell above/below

 A_i is the area of the top/bottom facet of the ith cell

 q_i is the magnitude of the net flux/Darcy velocity in the ith cell

Inter-cell average linear velocities are estimated from the Darcy velocities:

$$v_{ix} = \frac{q_{ix}}{\phi_i}, \quad v_{iy} = \frac{q_{iy}}{\phi_i}, \quad v = \frac{q}{\phi_i}v = \frac{q}{\phi_i}$$

where:

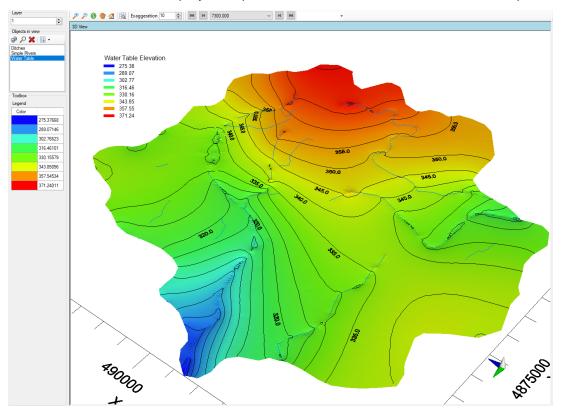
v is the average linear velocity (which can be a component flux or the magnitude as defined above)

q is the flux (which can be a component flux or the magnitude as defined above)

 ϕ_i is the effective porosity of the ith cell

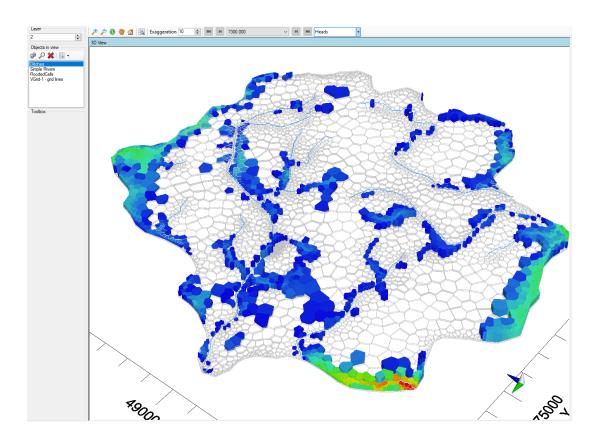
Water Table

The water table is the surface represented by the calculated head in the uppermost active cell in the simulation. In the 3D view, the Water Table is displayed as a surface object, and as such has style settings similar to Surfaces (for more details on these options, see <u>Style</u> <u>Settings: Surfaces</u>. If your model is Transient, you can adjust the output time as explained above, and the Water table display will update to reflect the new values for that output time.



Flooded Cells

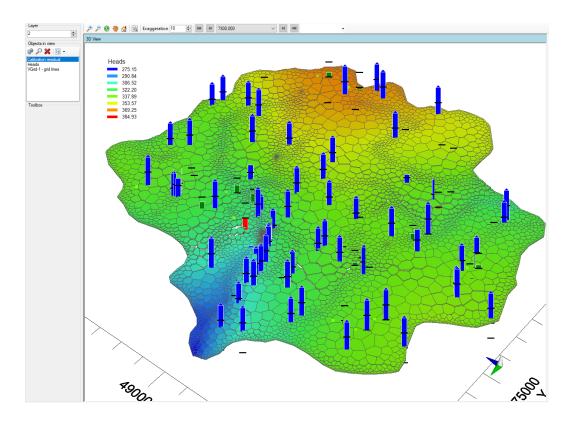
At the View Maps step, you can view "flooded" cells, which are the collection of cells intersecting the simulated water table that have simulated head values above the top of the model. The cells can be displayed as a solid color (by default) or using a color ramp based on the amount of flooding (i.e. simulated head - model top):



Flooded cells indicate the location and amount of flooding in the model which can be useful during model development as it may indicate that model parameters (such as conductivities, recharge, boundary conductances, etc.) require adjusting if flooding is simulated in unexpected areas of the model.

Residuals

If your model included observations, you can view residuals relative to a target residual as error bars with various <u>settings</u> at the View Maps step, as described in the section on <u>3D</u> <u>Gridded Data</u>.



Calculation of Residuals

In Visual MODFLOW Flex, residuals are expressed as the difference between the simulated value and the observed value. For example, the heads residuals are calculated as follows:

$$r = h_{calc} - h_{obs}$$

where:

r is the residual value

 h_{calc} is the model-calculated value

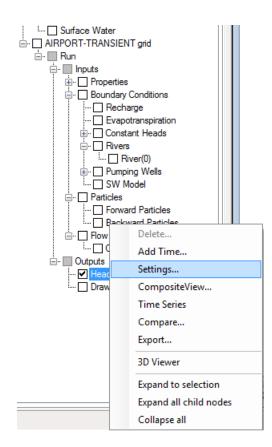
 h_{obs} is the observed value

When displayed in Visual MODFLOW Flex, residuals are compared to target values which can be set per observation or globally.

Adjusting Style Settings

You can adjust the style settings of object in the 3D view at the View Maps step as described in section on <u>Style Settings</u>.

First sure make the desired object is selected and visible in the Viewer. Then right-click on the desired property group in the tree as shown below and select `Settings`

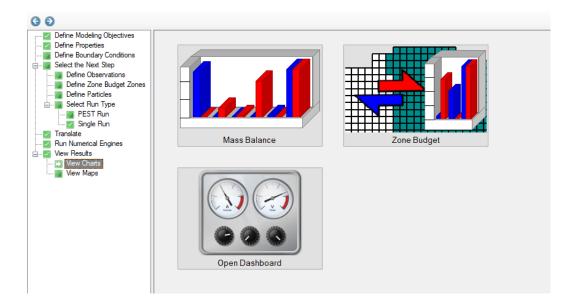


Exporting Outputs.

Outputs can also be exported in a variety of formats. Please see the section on Exporting Files for more details.

11.10.2 View Charts

Visual MODFLOW Flex, upon completing a successful model run, you can view several different types of charts to review your results and to facilitate model calibration.



Calibration Dashboard

The <u>Calibration Dashboard</u> is multi-component tabulation and charting view that is contained in its own tab. The dashboard consists of:

- a **table** of observations and associated modeling results that can be dynamically filtered and sorted,
- a statistics panel that dynamically calculates various calibration-related <u>statistics</u> of data visible in the table and in the charts
- charting area that can contain one or more of the following chart types:
 - Calc. vs obs. chart: scatter plot comparing calculated values (y-axis) versus corresponding observations (x-axis)
 - Time Series chart: line series plot of simulated results over and observed values vs time

Zone Budget

The <u>ZoneBudget Charts</u> include a set of charts that present data from Zone Budget runs:

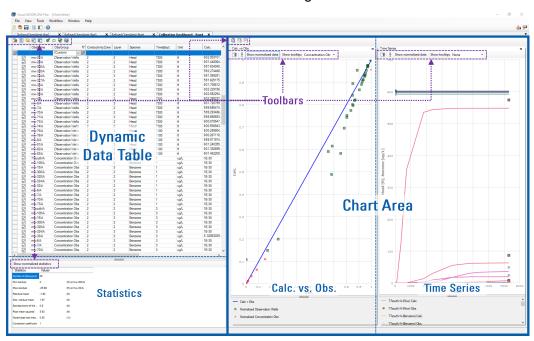
- **Percent Discrepancy** plots the temporal changes in the Flow Mass Balance for the selected zone (total flow IN minus total flow OUT) expressed as a percentage of the total flow in the zone.
- **IN OUT** plots the temporal change in the Flow Mass Balance for the selected zone (total flow IN minus the total flow OUT).
- **Time Series** plots the temporal flows IN and OUT of the selected zone through the individual sources and sinks (flow boundary conditions and storage).
- **Time Steps** plots a bar chart of the flow IN to the system and the flow OUT of the selected zone through the individual sources and sinks (flow boundary conditions and storage) for selected Output Times.

Note: this button is disabled if the run did not include ZoneBudget at the <u>single run</u> (select engines) step.

11.10.2.1 Calibration Dashboard

The calibration dashboard is a standalone multi-component view in Visual MODFLOW Flex that allows you to dynamically filter and plot both observed and simulated values for comparison, calibration, and evaluation purposes.

Layout



The calibration dashboard consists of the following elements:

- a **dynamic data table** of observations and associated modeling results that can be dynamically filtered and sorted,
- a statistics panel that dynamically calculates various calibration-related <u>statistics</u> of data visible in the table and in the charts
- a chart area that can contain one or both of the following chart types:
 - <u>Calc. vs Obs.</u>: scatter plot comparing calculated values (y-axis) versus corresponding observations (x-axis)
 - o *Time Series*: line series plot of simulated results over and observed values vs time
- A set of **toolbars** in each element that provides related controls

Each of the elements can be resized or hidden/shown using the following controls. Elements can be resized by clicking and dragging the bars that separate them and shown or hidden using the collapse (show/hide) buttons:



Dynamic Data Table

The dynamic data table displays data from all observation groups including observation data, equivalent simulation data, and associated metrics. Following a successful model run, Visual MODFLOW Flex will calculate simulated equivalent values for each observation, extract associated time series data from the simulation for each observation location/observation type, and calculate residuals and normalized values. Data from each observation group is then written to a tab separated variable file (.TSV) with a set number of fields. The TSV file contains two header rows, and is organized in fields (columns) and records (rows).

Headers

The first header row in a TSV file specifies field types:

- SetFilter fields contain descriptive metadata about the observation location that can be used to group or separate data;
- RangeFilter fields contain metadata describing the location of the observation in space and time;
- Unit fields contain the unit type for Value fields
- Value fields contain values for observations, calculated values, residuals, target residuals, and normalized values

The second header row in a TSV file specifies field names as described below.

Fields

The following fields are included in each TSV file:

- Visibility: a field with checkboxes that control whether the record is visible (or not) in charts in the chart area (check = visible, unchecked = hidden)
- ObsName: the name of observation well (including well screen id) or gage location [SetFilter]
- **ObsGroup**: the name of the well observation group or gage type [SetFilter]
- X[*unit*]: x-coordinate of the observation location, specified in project length units [RangeFilter]
- Y[*unit*]: y-coordinate of the observation location, specified in project length units [RangeFilter]
- **Z**[*unit*]: z-coordinate of the observation location, specified in project length units [RangeFilter]

- ConductivityZone: the conductivity property zone of the observation location [SetFilter]
- Layer: model layer of the observation location [SetFilter]
- GageType: type of location measured (e.g. boundary condition type) [SetFilter]
- GageMeasurement: measured parameter (e.g. volumetric flow, head) [SetFilter]
- Species: measured parameter (e.g. head, solute species) [SetFilter]
- **Time**[*unit*]: [RangeFilter]
- Unit: the measurement unit for observed, calculated, residual, and target values (e.g. m, m³/d, mg/L) [Unit]
- Calc.: calculated (simulated) values [Value]
- Obs.: observed values [Value]
- Residual: residual values [Value]
- TargetResidual: specified target residuals [Value]
- NormalizedCalc.: normalized calculated (simulated) values [Value]
- NormalizedObs.: normalized observed values [Value]
- NormalizedResidual: normalized residual values [Value]
- NormalizedTargetResidual: normalized target vales [Value]

One calculated value will be included for each distinct observation that occurs within an active model cell. For observations that do not coincide exactly with model spatial and temporal discretization, calculated outputs are linearly interpolated first in space (based on values from the nearest neighboring cells) and then in time using spatially interpolated values from the times steps that precede and follow the observation. Calculated values without corresponding observations will also be included as separate values for each output time specified in the output control settings for heads and budget-related outputs outputs, as applicable. Normalized values are dimensionless and the calculation of normalized values is described in the calibration statistics discussion. The first row in the table includes controls for filtering the data.

Toolbar

The following controls are available for the tabulated data:

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- 🔀 Clear all filters: clears any filters applied to the data
- **Choose Columns**: opens a window that allows you to choose which fields are shown in the table
- Some open Data Folder: opens the data subfolder containing the TSV files in the model data folder
- Copy Selected Rows to Clipboard: copies selected table rows to the clipboard for use in other applications

- Copy All to Clipboard: copies all table rows to the clipboard for use in other applications
- M Check All: toggles the visibility of all table row data in the charts to visible/on
- D Uncheck All: toggles visibility of all table row data in the charts to hidden/off
- **W** Invert Selection: inverts the selection of all table rows in the charts
- Check/Uncheck selected Rows: checks or unchecks selected table rows in the charts

Filters

The first row in the table is a blank row that allows you to filter the data. When data are filtered, the rows that meet the filter criteria will be shown in the table and charts, and data that do not meet the criteria are hidden. To filter records based on values in a given field, click in the desired field and make use the following controls:

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- Type: type a value in the field filter entry to filter to show only values that start with the typed value
- Dropdown: click the dropdown button to show a list of unique values. Selected values will be shown and all other values will be hidden. The dropdown also includes filters based on the field type:
 - Numeric fields can be filtered using one or more relations to a specified value (equals, does not equal, greater than, greater than or equal, less than, less than or equal, between, or a custom filter)
 - Text fields can be filtered using one or more relations to a specified string (equals, does not equal, begins with, ends with, contains, does not contain, or a custom filter)
- **Clear Filter**: clears any filters on the field

You can clear all filters by using the the clear filter (22) button at the far left side of the filter row.

Statistics

The statistics panel includes a list of <u>calibration statistics</u> that are commonly used when evaluating model results. These statistics are based on which data rows are shown in the table (i.e. not filtered) and set to visible (i.e. the visibility field is checked on). The following statistics are included:

Number of observation points

- Minimum (absolute value) residual
- Maximum (absolute value) residual
- Residual mean
- Absolute residual mean
- Standard error of the estimate
- Root Mean Squared
- Normalized Root Mean Squared
- Correlation Coefficient

Each of these statistics is described in the <u>calibration statistics</u> section. The "Show normalized statistics" button allows you to toggle whether the statistics are calculated using actual values or <u>normalized</u> values.

Chart Area

The chart area in the dashboard allows you to display either or both of the charts discussed below.

Toolbar

The following controls are available for the chart area:

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- I Choose Charts: opens a window that allows you to choose which charts are shown
- Symbol Settings: opens the symbology window for the Calc vs. Obs. chart.
- Market Time Series Settings: opens the symbology window Time Series chart.

Symbology Window

The symbology window allows you to define the symbology of the applicable chart.

😂 Symbology				_		\times
Group field ObsGroup	•					
Label	Symbol	Symbol color				
Riv:VolumetricFlow	Circle	128, 0, 51, 255	\sim	Observation Wells		
Observation Wells	Square					
Concentration Obs	Diamond			+ Concentration Obs		
	-					
				Apply	Clos	
				лрру	CIUS	ic .

- Group Field (Calc. vs. Obs. only): symbols can be grouped and defined based unique values in one of the <u>setFilter</u> fields in the data table (e.g. observation location name, observation group, conductivity zone, model layer, etc.)
- Label: symbol labels based on the unique values in the grouping field. Note that the Time Series chart are only grouped by observation location (ObsName field)
- **Symbol**: shape of the symbol (circle, square, diamond, pentagon, hexagon, pyramid [triangle], pentagram [star])
- Symbol color: color of the specified symbol (red, green, blue, alpha/opacity)

Calculated versus Observed Calibration Chart (Calc. vs. Obs)

The Calculated vs. Observed Chart consists of a scatter plot representing the comparison between the calculated and observed values shown in the dynamic data table. This graph represents a comparison between the values calculated by the model (Y-axis), and the values observed or measured in the field (X-axis). The situation where all data points intersect the *Calc.=Obs.* line line on the graph represents an ideal calibration scenario, but it is not likely to happen when developing models of real-world sites. If data points appear above the *Calc.=Obs.* line, then the calculated values are larger than the observed values, and the Calibration Residual is positive, indicating that the model is over-predicting. If the data points are under the *Calc.=Obs.* line, then the calculated values are less than the observed values, and the Calibration Residuals are negative, indicating that the model is under-predicting. The chart below indicates the model is generally under-predicting head values.

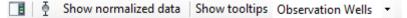


For simulations containing many different observation, types, locations, and times, the quality of the model calibration will likely be quite variable. Therefore, it is important to be able to evaluate the portions of the calibration to evaluate differences between calculated and observed values over different parameter types, spatial locations, and times. You can use the <u>filters</u> and visibility toggles in the <u>dynamic data table</u> to show (or hide) a subset of the data as appropriate. You can also <u>normalize</u> the data to plot different observation types spanning different ranges within a normalized range of 0 to 1.

The chart can optionally include error bars with +/- lengths corresponding to the target residual of each data point. An error bar for a given data point that intersects the *Calc.=Obs.* line indicates that the residuals are within the specified target residual range.

Toolbar

The following controls are available for the Obs. vs. Calc. chart:

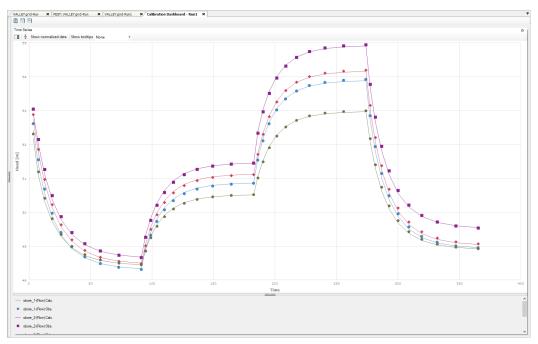


- **I** Toggle Legend Location: toggles whether the legend appears at the bottom of the chart or to the right
- Toggle Error bars: toggles whether or not to show error bars. Error bar length is based on the target residual (or normalized target residual if normalized values are shown).
- Show normalized data Show Normalized data: button to toggle whether regular/untransformed data or normalized data are displayed in the chart
- Show tooltips Observation Wells Show tooltips dropdown: allows you to select which series (including a single series, any series, or none) will include tooltips. Tooltips will be displayed for the single data point of the applicable series nearest to the mouse pointer when the pointer is within the chart area.

Time Series Plots

A Time Series graph plots the value of one or more selected variables over time. In groundwater flow and contaminant transport modeling, time-series graphs are used to evaluate and compare temporal trends in the calculated heads or volumetric flows at selected observation wells or gage points. In the Calibration Dashboard Time Series chart, observed values are plotted as discrete points, while corresponding simulated values are plotted as connected lines with same color. The situation where the lines representing simulated data intersect their corresponding observation data points represents an ideal calibration scenario, but it is not likely to happen when developing models of real-world sites. If data points appear above the corresponding simulated result line, then the calculated values are smaller than the observed values, and the calibration residual is negative, indicating that the model is under-predicting the parameter at that location and time. Conversely, if the data points are below the corresponding simulated result line, then the

calculated values are greater than the observed values, and the calibration residuals are positive, indicating that the model is over-predicting. The chart below is based on an exercise using PEST calibration and indicates that model results match observed values well.



For simulations containing many observations of different types, locations, and times, the quality of the model calibration will likely be quite variable and data may not fit neatly on the plot. Therefore, it is important to be able to visualize various subsets of the data to evaluate time series data of interest. You can use the <u>filters</u> and visibility toggles in the <u>dynamic data</u> table to show (or hide) desired subsets of the data. You can also <u>normalize</u> the data to plot different observation types spanning different ranges within a normalized range of 0 to 1.

The chart can optionally include error bars with +/- lengths corresponding to the target residual of each data point. An error bar for a given observation data point that intersects the simulation line indicates that the residuals are within the specified target residual range.

Toolbar

The following controls are available for the Time Series chart:

```
📑 🍦 Show normalized data Show tooltips Observation Wells 👻
```

- **I** Toggle Legend Location: toggles whether the legend appears at the bottom of the chart or to the right
- **Toggle Error bars**: toggles whether or not to show error bars. Error bar length is based on the target residual (or normalized target residual if normalized values are shown).

- Show normalized data Show Normalized data: button to toggle whether regular/untransformed data or normalized data are displayed in the chart
- Show tooltips Observation Wells Show tooltips dropdown: allows you to select which series (including a single series, any series, or none) will include tooltips. Tooltips will be displayed for the single data point of the applicable series nearest to the mouse pointer when the pointer is within the chart area.

11.10.2.1.1 Calibration Statistics

Calibration Statistics are reported in the footer of the Calibration Plots window when the Calculated vs. Observed Scatter Graph is displayed. These statistics are calculated using the assumption that the calibration residuals are normally distributed. The individual statistics are described below:

Calibration Metrics

The following calibration statistical metric values are calculated by Visual MODFLOW Flex and presented in the Model Dashboard. All metrics are based on the data visible in the table and charts (i.e. not filtered and checked as visible):

Calibration Residual

The calibration residual (R_i) is defined as the difference between the calculated results (X_{cal}) and the observed results (X_{obs}) at selected data points ($i = 1 \rightarrow n$) as shown in the following equation:

$$R_i = X_{cal} - X_{obs}$$

where:

 X_{cal} is the calculated value from the model

 X_{obs} is the measured/observed value

The absolute value maximum and minimum residuals at the selected observation points are also reported. When calculating residuals, it is important to compare values at the same location and point in time. Since observed values and calulated values from model simulations do not always perfectly coincide, when calculating residuals, Visual MODFLOW Flex bi-linearly interpolates the calculated values in space to the location of the observation within the given model layer and then linearly interpolates these values in time to match the time of the observation. Calculated values are <u>not</u> interpolated between layers. As such, groundwater models should ideally be designed so that the gaps in space and time between

observations and corresponding model outputs are relatively small to minimize inaccuracies due to interpolation.

Residual Mean

The residual mean (\overline{R}) is a measure of the average residual value defined by the equation:

 $\bar{R} = \frac{1}{n} \sum_{i=1}^{n} R_i$

where:

n is the number of observations

 R_i is the ith residual

Please Note: there may be cases where over-calculated and under-calculated values will negate each other, and produce a value of the residual mean close to zero. This can lead to false interpretation of the model calibration - the residual mean should never be used by itself as a measure of the fit between the simulated results and the observed data.

Absolute Residual Mean

The absolute residual mean $(|\bar{R}|)$ is similar to the residual mean except that it is a measure of the average absolute residual value defined by the equation:

$$|\bar{R}| = \frac{1}{n} \sum_{i=1}^{n} |R_i|$$
where:

n is the number of observations

 R_i is the ith residual

The absolute residual mean measures the average magnitude of the Residuals, and therefore provides a better indication of calibration than the Residual Mean.

Standard Error of the Estimate

The standard error of the estimate (SEE) is a measure of the variability of the residual around the expected residual value, and is expressed by the following equation:

$$SEE = \sqrt{\frac{\frac{1}{n-1}\sum_{i=1}^{n} (R_i - \bar{R})^2}{n}}$$

where:

n is the number of observations

 R_i is the ith residual

 \bar{R} is the mean residual (described above)

Root Mean Squared

The Root Mean Squared error (*RMS*) is a measure of the variance of the model residuals and is defined by the following equation:

$$RMS = \sqrt{\frac{1}{n} \sum_{i=1}^{n} R_i^2}$$

where:

n is the number of observations

 R_i is the ith residual

Normalized Root Mean Squared

The Normalized Root Mean Squared (*NRMS*) is the RMS divided by the maximum difference in the observed head values, and is expressed by the following equation:

$$NRMS = \frac{RMS}{(X_{obs})_{max} - (X_{obs})_{min}} \cdot 100\%$$

where:

RMS is the Root Mean Square error (described above)

 X_{obs} is the measured/observed value

The NRMS is expressed as a percentage, and is a more representative measure of the fit than the standard RMS, as it accounts for the scale of the potential range of data values. For example, an RMS value of 1.5 will indicate a poor calibration for a model with a range of observed values between 10 and 20, but it will indicate an excellent calibration for a model with a range of observed values between 100 and 200. The NRMS value for the first model would be 15%, while the NRMS for the second model would be 1.5%. The NRMS values clearly indicate the second model provides a better fit between the calculated and observed values.

Correlation Coefficient

The Correlation Coefficient (*Cor*) is calculated as the covariance (*Cov*) between the calculated results (X_{cal}) and the observed results (X_{obs}) at selected data points divided by the product of their standard deviations. The correlation coefficient is calculated using the following equation:

$$Cor(X_{cal}, X_{obs}) = \frac{Cov(X_{cal}, X_{obs})}{\sigma_{cal} \cdot \sigma_{obs}}$$

where:

 X_{cal} is the calculated value from the model

 X_{obs} is measured/observed value

 σ_{cal} is the standard deviation of the calculated values from the model

 σ_{obs} is the standard deviation of the measured/observed values

Cov is the covariance of the calculated and observed values

The covariance is calculated using the following equation:

$$Cov(X_{cal}, X_{obs}) = \frac{1}{n} \sum_{i=1}^{n} (X_{cal} - \bar{X}_{cal}) (X_{obs} - \bar{X}_{obs})$$

where:

 X_{cal} is the calculated value from the model

 X_{obs} is measured/observed value

 \bar{X}_{cal} is the mean of the calculated values from the model

 \bar{X}_{obs} is the mean of the measured/observed values

The average values \bar{X}_{cal} and \bar{X}_{obs} are calculated as follows:

$$\bar{X}_{cal} = \frac{1}{n} \sum_{i=1}^{n} X_{cal(i)} , \ \bar{X}_{obs} = \frac{1}{n} \sum_{i=1}^{n} X_{obs(i)}$$

where:

n is the number of observations

 X_{cal} is the calculated value from the model

 X_{obs} is measured/observed value

The standard deviations σ_{cal} and σ_{obs} are calculated as follows:

$$\sigma_{cal} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} \left(X_{cal(i)} - \bar{X}_{cal} \right)^2}, \quad \sigma_{obs} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} \left(X_{obs(i)} - \bar{X}_{obs} \right)^2}$$

where:

n is the number of observations

 X_{cal} is the calculated value from the model

 X_{obs} is measured/observed value

 \bar{X}_{cal} is the mean of the calculated values from the model

 \bar{X}_{obs} is the mean of the measured/observed values

Correlation coefficients range in value from -1.0 to 1.0 and determine whether two ranges of data move together – that is, whether large values of one data set are associated with large values of the other data set (positive correlation), whether small values of one data set are associated with large values of the other data set (negative correlation), or whether values in both sets are unrelated (correlation near zero).

Normalized Values

Visual MODFLOW Flex allows you to normalize (rescale) observed and simulated data values so that different observation/measurement types spanning different orders of magnitude can be simultaneously compared. Values are normalized to the range of values (ΔX_G) within each observation group:

$$\Delta X_G = X_G^{max} - X_G^{min}$$
$$X_G^{max} = max(X_{obs}, X_{cal})$$
$$X_G^{min} = min(X_{obs}, X_{cal})$$

where:

 ΔX is the range of (observed or calculated) values

 X_{G}^{max} is the maximum (observed or calculated) value in the observation group

 X_{G}^{min} is the minimum (observed or calculated) value in the observation group

 X_{obs} is the measured/observed value of the current observation/measurement group

 X_{cal} is the calculated/simulated value of the current observation/measurement group

The scale (κ_G) and translation (λ_G) factors for normalization are based on the range of values and adjusted to avoid division by zero:

$$\kappa_{G} = \begin{vmatrix} \Delta X_{G} > 0 & : & \frac{1}{\Delta X_{G}} \\ \Delta X_{G} = 0, X_{G}^{max} \neq 0 & : & \frac{1}{|X_{G}^{max}|} \\ \Delta X_{G} = 0, X_{G}^{max} = 0 & : & 1 \end{vmatrix}$$

$$\lambda_{G} = \left| \begin{array}{ccc} observed & : & X_{G}^{min} \\ calculated & : & X_{G}^{min} \\ \\ residual & : & 0 \\ target\,residual & : & 0 \end{array} \right.$$

Observed and calculated values are translated and scaled, while residuals and target residuals are just scaled:

$$X'_{i} = \kappa_{G}(X_{i} - \lambda_{G})$$
$$r'_{i} = \kappa_{G}(X_{i})$$

where:

 X'_{i} is the ith normalized observed or calculated value in the observation group

 r'_i is the ith normalized residual or target residual

In Visual MODFLOW Flex, the values, whether observed or calculated (simulated) are normalized/rescaled using both observed and calculated values so that the rescaling transformations are consistent and linear and fall within a range of 0 to 1.

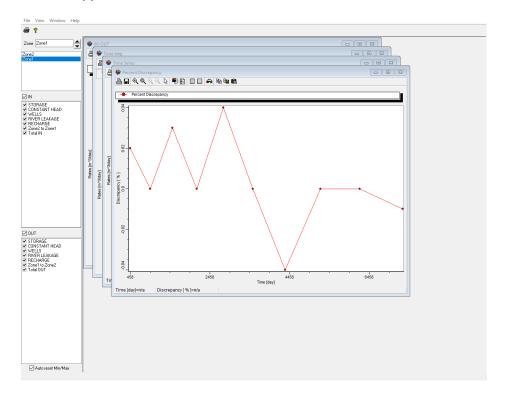
11.10.2.2 ZoneBudget Charts

ZoneBudget is a program developed by the U.S. Geological Survey to calculate water budgets for user-defined zones in the model. The user-defined ZoneBudget zones are created during the Define ZoneBudget Zones step (<u>finite difference</u> or <u>unstructured</u>) workflow step. The Zone Budget program calculates the flow mass balance for each user-defined zone.

Flow Zone Budget Graphs

The Flow Zone Budget Graphs plot the flow rates of water entering and leaving the userdefined zones through the flow boundary conditions, from aquifer storage, and through other user-defined zones.

To plot the Zone Budget Graphs, select the View Charts workflow step, click the Zone Budget Button on the upper left corner of the Chart view, and a Zone Budget: MODFLOW window will appear as shown below:



There are four different Flow Zone Budget Graphs:

- **Percent Discrepancy** plots the temporal changes in the Flow Mass Balance for the selected zone (total flow IN minus total flow OUT) expressed as a percentage of the total flow in the zone.
- **IN OUT** plots the temporal change in the Flow Mass Balance for the selected zone (total flow IN minus the total flow OUT).
- **Time Series** plots the temporal flows IN and OUT of the selected zone through the individual sources and sinks (flow boundary conditions and storage).
- **Time Steps** plots a bar chart of the flow IN to the system and the flow OUT of the selected zone through the individual sources and sinks (flow boundary conditions and storage) for selected Output Times.

Please Note: With both the Time Steps and the Time Series graphs, it is important to remember that these graphs present the rate(s) at a point (or points) in time, and not the cumulative volume at a point in time.

Controls

On the left-hand side of the Zone Budget: MODFLOW window is a list of the Zone Budget zones available for the current model. The Zone Budget graphs described above will display the Zone Budget data for the selected Zone Budget zone.



The Zone List Box Control

The Zone Control indicates the current Zone for the active charts and the list box below shows all available ZoneBudget zones in the model. Clicking directly on a Zone in the list will switch to that Zone.

The IN/OUT List Box Controls

The IN list contains each of the possible source terms which may contribute flow to the selected Zone Budget zone, while the OUT list contains each of the possible sink terms which may divert flow out of the selected Zone Budget zone.

The checkboxes beside each term can be used to add or remove the individual source and sink terms from either the Time Series graph or the Time step graph.

The group checkboxes will add or remove the entire IN/OUT group.

The Percent Discrepancy graph and the IN-OUT graph consider only the total flow into and out-of the entire system as a whole. As a result, the settings for the individual IN and OUT terms do not influence the results and appearance of these graphs.

Note: By convention, Zone Budget considers mass balance from the perspective of the groundwater system. For example, the IN term for River Leakage represents the river leakage INTO the groundwater system.

Arranging the Graphs

Each of the graphs can be maximized to occupy the entire Zone Budget window by clicking the maximize button in the top right-hand corner of each graph window. Alternately, the graphs can be tiled in the Zone Budget window by selecting Window/Tile from the top menu bar.

12 Surface Water Workflow

Visual MODFLOW Flex provides a separate workflow within the numerical modeling workflow for developing a representation of surface water features independent of the grid. With this conceptual approach, you define a network of connected linear and areal surface water features such as streams, ditches, diversions, and canals or lakes and ponds, respectively. These surface water features are defined using vector representations (lines and polygons) built within a topology that defines both the connections between these features as well as their individual attributes.

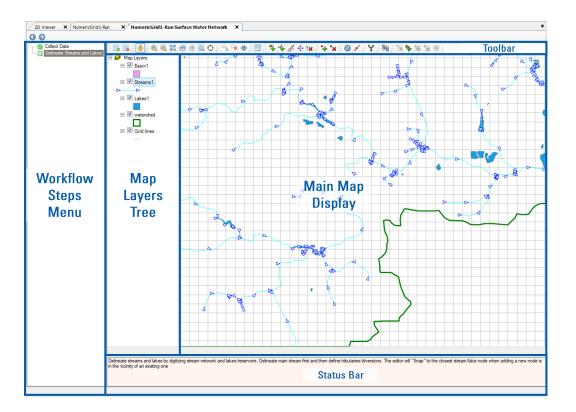
The steps to develop the Surface Water Workflow is described in the sections of this Chapter as follows:

- Interface Layout: describes the layout of the Surface Water Workflow, general controls, and workflow steps
- <u>Delineate Streams and Lakes</u>: describes the process to delineate streams and lakes in the surface water workflow, which involves defining the spatial features and topology of the surface water network
- Surface Water Network Data: describes the attribute data of streams and lakes

12.1 Interface Layout

The surface water workflow has a unique interface within the Visual MODFLOW Flex that includes its own layout. The layout consists of the following components:

- Workflow Steps Menu
- Map Layers Tree
- Toolbar
- Main Map Display
- Status Bar



Workflow Steps Menu

The Surface Water workflow is divided into two steps. Both steps include a light-weight Geographic Information System (GIS) interface that allows you to visualize and manipulate the input data required to develop the surface water network for inclusion in a <u>Numerical</u> <u>Modeling Workflow</u>.

To navigate between the two steps, you can either click on directly on the name of the step

or use the previous \bigcirc or next \bigcirc buttons.

Collect Data

At this step in the workflow, you collect the data you want to use to build the surface water portion of the model. The surface water workflow is data driven. This means that you first need to "collect" the appropriate data objects in order to use these at a particular step in the workflow. Data objects can be "collected" by importing data layers or creating them. By default, the model gridlines will be added to the view.

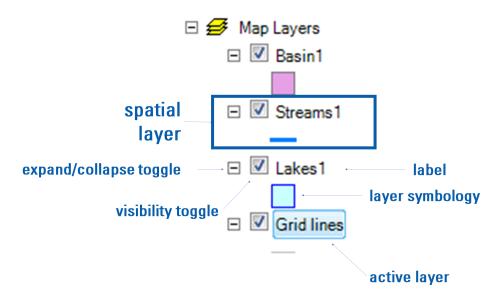
Delineate Streams and Lakes

At this step in the workflow, you delineate and define the surface water drainage network which consists of a series of connected directed segments and (optional) lakes. Upon reaching this step for the first time, several empty layers will be added that will be used to define the stream segments and lake areas in the surface water network. For more information, please refer to the section on **Delineate Streams and Lakes**.

Map Layer Tree

Spatial layers added to the map, will be displayed in the Map Layer Tree. Each added spatial layer includes:

- a label,
- layer symbology,
- a toggle to expand/collapse the symbology, and
- a visibility toggle that will show or hide the layer in the map display.

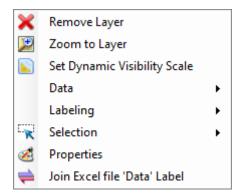


Active Layer

The active layer is the focus of many tools in the map view. To make a layer the active layer, simply click on the label. As shown above, the active layer will be highlighted in blue.

Context Menu

Right-clicking on the a layer will provide additional options as follows:



- Remove Layer: removes a layer from the map
- Zoom to Layer: zooms the map to the extents of the active layer
- Set Dynamic Visibility Scale: allows you to control if the layer will be show above/below the current zoom extent
- Data: allows you to export the active layer
- Labeling: allows you to setup and show labels for the active layer
- Selection: provides controls for the selected features in the active layer
- **Properties**: allows you to set the layer symbology
- Join Excel file 'Data' Label: allows you to join attributes from an Excel file based on a join field.

Warning: Do not delete any of the automatic layers (i.e. Basin1, Streams1, Lakes1, and Gages1) this will corrupt the Surface Water Network

Toolbar

The toolbar provides the following controls to interact with the data in the main map display:

| 🚾 🗠 | 🍓 | 🔍 🤐 😂 🐼 | 🗠 🐵 📖 | 🐾 🍁 🌽 💠 🗛 | 📟 | 🎋 🛊 🖌 🖉

Navigation and General Map tools

The following tools are related to navigating and interacting with data layers displayed in the main map display:

- Add Layer: adds a shape or raster data layer to the map
- Bemove Layer: removes the active layer from the map
- 🥮 Pan: shifts the map view by clicking and dragging the map to pan
- Soom In: incrementally zooms into the map at the selected area
- 🧟 Zoom Out: incrementally zooms out from the map at the selected area
- Zoom to Extents: zooms to the combined extents of all layers

- Soom to Previous Extents: zooms to the previous map extents
- Zoom to Next Extents: zooms to the next map extents, if the zoom to previous button was clicked
- Soom to Layer: zooms to the extents of the active layer
- Select: selects features from the currently active layer:
 - o left-click to select a single feature,
 - o click and drag to select multiple features,
 - o hold the [SHIFT] key to add to the selection
- **Show Information**: displays information about the attributes of shapes at the location clicked in the map

Surface Water Network Editing Tools

The following tools are related to delineating and editing surface water features and are enabled/disabled based on the active layer:

- Bhow Attributes: displays the <u>Surface Water Network Data</u> table
- Add Layer to Network: allows you to select a shapefile to automatically add all of its features to the network in the active layer
- Add Shape to Network: allows you to draw a new shape to the active layer
- Z Edit shape: allows you to edit features in the active layer (moved nodes will maintain topology and connected nodes will move synchronously)
- **Move Vertex**: allows you to move vertices in the active layer (moved nodes will not maintain topology)
- **IX Delete Segment**: allows you to delete a shape from the active layer
- Add Vertex: allows you to add vertices to a selected segment
- **Delete Vertex**: allows you to delete vertices from a selected segment
- 10 Reverse Segment: allows you to flip the flow direction of a selected segment
- **Split Segment**: allows you to split a stream segment at a specified location along its path
- Validate Junctions: adds symbols representing the network topology for network connectivity <u>validation</u>
- Realize: generates/updates a layer that includes all of the grid cells that will be included in the SFR package based on the current stream network (available in numerical workflows only
- 🔭 Select Gage: opens the Gage Editor dialog for the selected gage
- Add Stream Reach Gage: allows you to add a stream reach gage to the selected stream segment
- Add Lake Gage: allows you to add a stream reach gage to the selected stream segment
- 🔀 Delete Gage: allows you to delete gages from the network
- It Move Gage: allows you to move a gage

The tools are described in more detail in the **Delineate Streams and Lakes** section.

12.2 Delineate Streams and Lakes

At this step in the Surface Water workflow, you can delineate streams and lakes in the surface water network. Upon arriving at this step, Visual MODFLOW Flex will automatically add four layers:

- Streams1: layer for adding stream segments in the surface water network
- Lakes1: layer for adding lakes connected in the surface water network
- Basin1: layer for the watershed boundary. (Not currently necessary to complete).
- Gridlines: gridlines from the numerical model

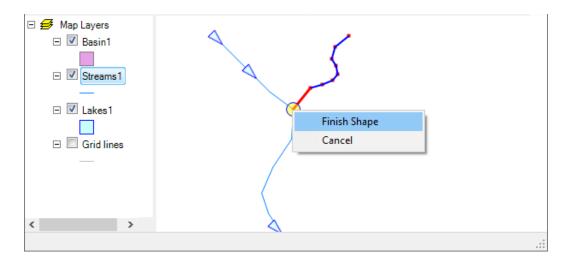
Adding Streams/Lakes

There are two methods to add streams or lakes to the surface water workflow to build the surface water network: digitizing individual features or adding an entire polyline (or polyline) shapefile with stream segments (or lakes) to automatically/sequentially add features within the shapefile to the network.

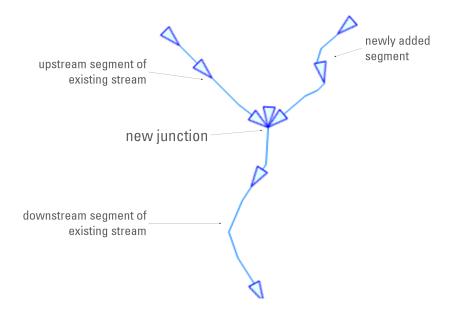
Pigitize Stream or Lake

To digitize a new stream segment:

- Select the Streams1 layer to make it the active layer.
- Click the Add Shape to Network button (^{**}) and begin drawing a new segment in the downstream direction
- The last vertex of the stream segment is added by right-clicking and selecting finish to complete the segment
- If you want to connect the new stream segment to the surface water network (i.e. at a stream or lake), simply hover the mouse over an existing stream or lake at the desired junction point. Visual MODFLOW Flex will automatically snap the junction to the existing feature at the point denoted by a yellow circle on vertices or by a red circle along the line of the existing feature.



• If the segment is added along an intermediate point along the stream network, then the existing stream segment will be split into upstream and downstream segments at the junction.



The steps to digitize a lake are the same as for a stream segment, except that you must select Lakes1 as the active layer. Also, lakes will not split stream segments if they overlap and so should generally be digitized before streams.

👎 Add Shapefile to Network

You can add an entire shapefile to the surface water. To add stream segments from a polyline shapefile to the surface water network:

- Select the Streams1 layer to make it the active layer.
- Click the Import shape file button (^{*}) and select the desired polyline shapefile using the Open dialog

 Click OK and Visual MODFLOW Flex will automatically sequentially add each feature in the shapefile to the surface water network. Features will be added individually and snapped in the network.

Please Note: snapping is based on the zoom scale and will likely provide better results if you zoom in so that you can see the individual line segments that comprise the polylines. Adding a shapefile with many features to the network may take a while, please be patient.

Once Visual MODFLOW Flex has processed the input shapefile, a summary of the number of segments added to the stream network will be provided. If any of the added stream segments to be added violate the topological rules described below, then these segments will be skipped and the features will be listed by feature ID in the default text editor.

The steps to add a lake are the same as for a stream segment, except that you must select Lakes1 as the active layer.

Deleting Streams/Lakes

To delete a stream segment:

- Select the Streams1 layer to make it the active layer.
- Click the Delete Segment button (¹)
- Hover the mouse pointer over the segment to be deleted and it will be highlighted red
- Left click and you will be prompted if you want to delete the segment

Confirmation	\times
Are you sure you want to delete this segment?	
Yes No	

The steps to delete a lake are the same as for a stream segment, except that you must select **Lakes1** as the active layer.

Editing Streams/Lakes

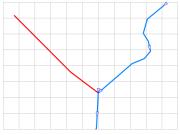
There are several tools available to edit the stream network as described below.

Warning: There is no undo function. Please edit shapes with caution

🌽 Edit Shape

You can edit a shapefile, including a stream or lake using the Edit Shape feature. To edit a feature within a shape:

- Select the layer to be edited in the Map Layers tree to make it the active layer
- Select the Edit Shape button (2/2) in the toolbar
- Hover over the feature to be edited and it will be highlighted red



• Double click on the feature and each of its vertices will be shown as blue squares



- Click and drag any vertex to move it.
- If the selected vertex to be moved is topologically shared with other/connected features (e.g. at the confluence of a stream, at a diversion point, or where a stream is connected to a lake), the shared vertices will also be moved.

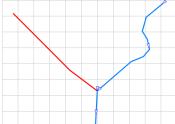
4 Move Vertex

You can move vertices in a shapefile, including a stream or lake using the Move Vertex feature. The steps are the same as Edit Shape, except that vertices having a shared topological connection with the moved vertex <u>will not</u> be moved along with it, breaking the topology. The Edit Shape and Move Vertex tools can be used in combination to edit/repair the network topology.

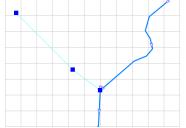
Hadd Vertex

You can add one or more vertices to a feature in a shapefile, including a stream or lake using the Add Vertex tool. To add a vertex to a feature within a shape:

- Select the layer to be edited in the Map Layers tree to make it the active layer
- Select the Add Vertex button (1+) in the toolbar
- Hover over the feature to be edited and it will be highlighted red



• Double click on the feature and each of its vertices will be shown as blue squares

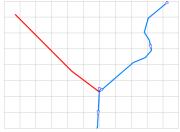


- Left click along the line where you wish to add a vertex
- You may also click and drag the vertices to move them

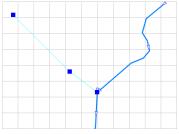
🗱 Delete Vertex

You can delete one or more vertices from a feature in a shapefile, including a stream or lake using the Delete Vertex tool. To remove a vertex from a feature within a shape:

- Select the layer to be edited in the Map Layers tree to make it the active layer
- Select the Add Vertex button (**) in the toolbar
- Hover over the feature to be edited and it will be highlighted red



• Double click on the feature and each of its vertices will be shown as blue squares

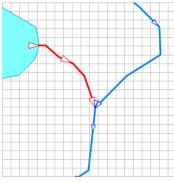


· Left click on the vertex/vertices you wish to delete from the selected feature

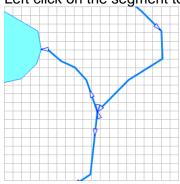
Reverse Segment

You can reverse the direction of a stream segment using the Reverse Segment tool. To reverse the direction of a stream segment:

- Select the layer to be edited in the Map Layers tree to make it the active layer
- Select the Reverse Segment button (1990) in the toolbar
- Hover over the feature to be edited and it will be highlighted red



· Left click on the segment to reverse its direction



Editing Attributes

You can view and edit stream and lake attributes by using the Attribute Table button. This will open the <u>Surface Water Network Data</u> table.

Network Topology

In order to simulate surface water flows in the SFR and LAK packages, the connections between the stream segments in the Streams1 layer and the lake areas in the Lakes1 layer must conform to the following rules:

- Stream segments must be oriented in the downstream direction (the flip tool may be used to make corrections)
- Lakes have no directional orientation
- Junctions are locations where stream segments and/or lakes connect. Valid junctions include the following scenarios:

- o Multiple (up to 10) upstream segments can connect to a single downstream or lake
- Multiple (up to 10) downstream stream segments can connect to a single upstream segment or lake a junction. In this case, one of the downstream segments must be designated as the outfall of the single upsteam segment (via the OUTSEG setting) and all other downstream segments will be considered as stream diversions subject to certain diversion requirements (via the IPRIOR option).
- Multiple upstream segments
- Lakes can have multiple (up to 10) upstream stream segments but only one downstream segment
 - Where a stream is upstream of a lake, the lake must be selected as its OUTSEG
 Where a steam is downstream of a lake, the lake must be selected as its IUPSEG
- The surface water network should not contain virtual stream segments (such those typically included in the National Hydrography Dataset [NHD] developed by the USEPA) located inside the footprint of lakes.

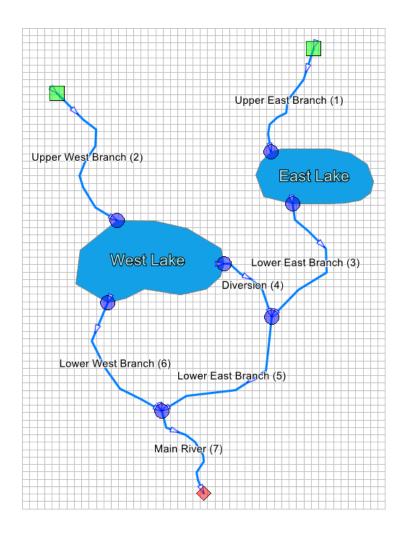
In general, the rules described above are enforced by Visual MODFLOW Flex as you add features to the surface water network, either individually (*) or if imported in bulk (*) as described above.

Network Validation 🚏

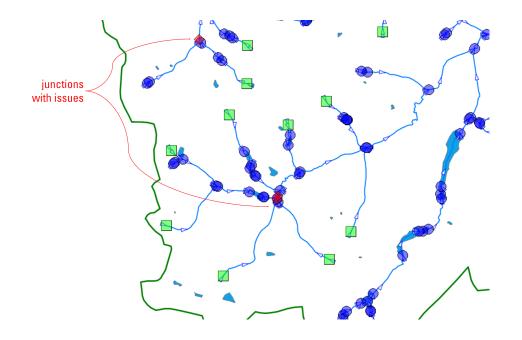
In some cases, the stream network may contain certain defects, particularly in the case of streams that have been imported in bulk. The Validate button in the toolbar is a useful tool to help you quickly visually inspect the stream network topology to verify that the stream network is correctly defined. Pressing the validate button (*) will overlay symbols on the junctions in the stream network as follows:

- Upstream Junctions with no tributaries are denoted by a green square
- Intermediate junctions that connect and upstream stream or lake to a downstream stream/lake are denoted by a blue circle
- Downstream Junctions with no outlets are denoted by a red diamond

The example shown below includes an example of a valid topology with no gaps in the connectivity of streams/lakes or inverted stream directions. In such cases a quick visual inspection using the validate button would quickly allow you to find and repair such defects in the network, using the <u>edit shape</u>, <u>move vertex</u>, and other functions, as appropriate.



The second example (below) demonstrates the validation of junctions in a natural stream channel that was imported and contains topological defects. The example demonstrates that visual inspection of the stream network has mostly correct topology and several stream segments with incorrect topology. In this particular case, the stream network contains small gaps and shorter stream segments with reversed flow directions.

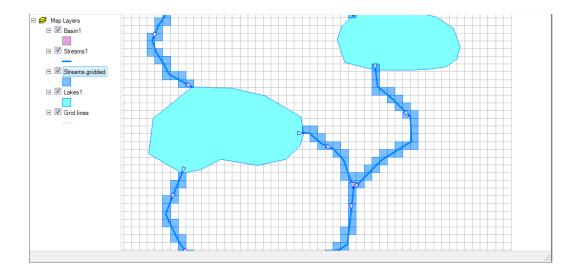


Realize Surface Water Network

In order to simulate surface water flows in the SFR and LAK packages, the surface water network must be converted from grid-independent vector features to grid-based datasets. If the Surface Water network workflow is part of a numerical run, then you can perform this conversion using the "realize" functions described below:

Realize Stream Segments

To realize the stream segments (i.e. prepare the layer for use in a MODFLOW model), first edit the segments using the tools described above and set the desired attributes in the <u>Surface Water Network Data</u> table. Once you are satisfied with the state of the stream segments, select the **Realize** button (\square) to convert the data in the Streams1 layer to the model grid. This will add the **Streams.gridded** layer to the Map Layers tree and the map if one is not present or update the layer if it already exists:



Realize Lakes

To realize lakes (i.e. prepare the layer for use in a MODFLOW model):

- Edit the Lakes1 layer using the tools described above,
- Open the <u>Surface Water Network Data</u> table by pressing the Attribute button (^{IIII}),
- Select the Lakes tab, and
- Press the "Realize lakes" button

The "Realize lakes" button will add each lake as a separate LAK package boundary condition in the numerical workflow with the appropriate index so that the topology will be preserved. For more information, please see <u>Surface Water Network Data</u>.

12.3 Surface Water Network Data

In Visual MODFLOW Flex, the SFR Package requires a more complex set of inputs than the other boundary conditions and as such is defined in its own <u>worflow</u>. Surface Water inputs are grid independent and are based on a set of parameterized vector geometries that define the surface water network consisting of connected/directed stream segments and optional lake polygons. Inputs for each of these is defined in this section.

Please Note: The collection of inputs in the SFR package is rather complex and interconnected, therefore a thorough review of the SFR2 input requirements as <u>documented</u> by the USGS is highly recommended before completing model development with the SFR package. A review of the GAGE package <u>documentation</u>, which facilitates the simulation and extraction of various types of surface water data including stage and flows is similarly recommended.

The Surface Water network consists of Streams and, optionally, Lakes. The input data required for Streams and Lakes are available in separate tabs in the Surface Water Network Data table. Supported inputs for each are described below.

Stream Segment Properties

A brief summary of supported inputs is presented below:

Name Type Surface Water Network SFR2 ✓			•								
		~ Ti	Time interval			nel (6a) Upstre	5)				
			Start time	End time	HCOND		THICKM	ELEV	WIDTH	DEPTH	THTS
treams La	kes Gages	•	. 0	31	•	0.0001	1	0	1	1	0.3
Index	Name		31	60		0.0001	1	0	1	1	0.3
			60	91		0.0001	1	0	1	1	0.3
1	Upper Right Bran		91	121		0.0001	1	0	1	1	0.3
▶ 5	Lower Right Bran		121	152		0.0001	1	0	1	1	0.3
3	Lower Right Bran		152	182		0.0001	1	0	1	1	0.3
4	Diversion (4)		182	213		0.0001	1	0	1	1	0.3
2	Upper Left Branc		213	244		0.0001	1	0	1	1	0.3
7	Main River (7)		244	274		0.0001	1	0	1	1	0.3
6	Lower Left Branc		274	305		0.0001	1	0	1	1	0.3
			305	335		0.0001	1	0	1	1	0.3
			335	366		0.0001	1	0	1	1	0.3
					<						
streams		12	time interva	la.	-						

Static Stream Segment Properties

The following parameters are defined per stream segment for the duration of the simulation period:

- Index: read-only unique integer identifier for each stream segment calculated by Visual MODFLOW Flex. The index must increase in the downstream direction so that all segments upstream of a given segment in the stream network stream have a lower index value.
- Name: an optional text input name for the stream segment that can be used to label the segment in Flex viewers and in the raw MODFLOW SFR input file

Dynamic Channel Segment Properties

There are several groups of parameters that are defined once per stress period each with a different spatial scope.

Stream Input/Output Options (Dataset 5)

The following parameters are defined once per stress period for <u>all</u> segments in the stream network (Dataset 5):

- IRDFLG: A flag to repeat/print input values in the MODFLOW listing file with the following options
 - o No listing: values will not be printed in the listing file
 - $\circ\,$ List upstream info: values from the upstream end of the segment will be repeated/printed in the listing file
 - List downstream info: values from the downstream end of the segment will be repeated/printed in the listing file
- IPTFlag: A Boolean flag to print values in the Budget File whenever the "Save Budget" option is specified (i.e. F.Term is checked) in the <u>Output Control</u> options.

Stream Segment Topology and Flow Data (Dataset 6a)

The following parameters are defined per stress period for <u>each</u> segment in the stream network :

- **ICalc**: a flag to specify the method by which the stream depth will be estimated (see <u>depth calculation</u>):
 - Specified Depth (ICalc=0): the stream depth will be specified at both the upstream and downstream end of the segment and linearly interpolated to the midpoint of each reach
 - Variable depth (ICalc=1): the stream depth will be estimated based on the estimated discharge at the midpoint of the stream and Manning's equation.
- **OUTSEG Index**: the stream index downstream of the current stream segment. Note that Visual MODFLOW Flex will automatically determine the default OUTSEG index value based on the network topology. Stream segments are indicated by using the positive value of the stream index and Lakes are indicated by using the <u>negative</u> value of the lake index. If more than one segment is downstream, the index of the first segment added will be used and any other downstream segments will be assumed to be connected <u>diversions</u>.
- **IUPSEG Index**: the stream index upstream of the current stream segment used if and only if the current stream is a <u>diversion</u>, otherwise a value of 0 should be used. Note that Visual MODFLOW Flex will automatically determine the value for IUPSEG based on the network topology.
- **IPrior**: a flag to specify how flows should be diverted to the current stream segment, used if and only if the current stream is a diversion, otherwise the value is ignored:
 - Reduce to available (IPRIOR=0): all available flow at the end of the last reach of a segment up to the rate specified will be diverted from the segment. If flow in the stream is less than the specified diversion, all available flow in the stream will be diverted, and none will remain in the channel.
 - *Reduce to None (IPRIOR=1)*: the specified diversion will only occur if flow in the stream is greater than that of the diversion. If flow is less than the specified diversion, then no flow is diverted and all flow remains in the channel.
 - Fraction of Available (IPRIOR=2): a specified fraction of the available flow will be diverted.
 - Divert Excess (IPRIOR=3): all flow in excess of a specified rate will be diverted.

- **FLOW**: volumetric rate of streamflow (L³/T) entering or leaving the upstream end of a stream segment (i.e. the first reach) as follows:
 - o If the current stream is a *headwater* stream (i.e. the current segment has no tributaries), FLOW defines the total inflow to the first reach of the segment. The value can be any number ≥ 0.
 - If the current stream is a *tributary* stream (i.e. the current segment has at least one tributary and is not itself a diversion), FLOW defines additional specified inflow to or withdrawal from the first reach of the segment (that is, in addition to the discharge from the upstream segment of which this is a tributary). This additional flow does not interact with the ground-water system. For example, a positive number might be used to represent direct outflow into a stream from a sewage treatment plant, whereas a negative number might be used to represent pumpage directly from a stream into an intake pipe for a municipal water treatment plant.
 - If the current stream is a *diversionary* stream and the diversion is from another stream segment (i.e. IUPSEG for the current segment > 0), FLOW defines the streamflow diverted from the last reach of stream segment IUPSEG into the first reach of this segment. The diversion is computed or adjusted according to the value of <u>IPrior</u>.
 - If the stream is a *diversionary* stream, and the diversion is from a lake (i.e. IUPSEG for the current segment < 0), FLOW defines a fixed rate of discharge diverted from the lake into the first reach of this stream segment (unless the lake goes dry) and flow from the lake is not dependent on the value of <u>ICALC</u>. However, if FLOW = 0, then the lake outflow into the first reach of this segment will be calculated on the basis of lake stage relative to the top of the streambed for the first reach using one of the methods defined by ICALC.
- Runoff: volumetric rate of overland flow into the stream segment (L³/T)
- ETSW: volumetric rate of direct evapotranspiration from the stream segment (L³/T)
- **PPTSW**: volumetric rate of direct precipitation into the stream segment (L³/T)
- ROUGHCH: the value of Manning's roughness coefficient in the stream segment
- CDEPTH: not used

Upstream Stream Segment Properties (Dataset 6b)

The following parameters are defined per stress period for the upstream end of <u>each</u> segment in the stream network:

- **HCOND**: the hydraulic conductivity of the bed at the upstream end of the current segment [L/T]
- **THICKM**: the thickness of the stream bed sediments at the upstream end of the current segment [L/T]
- ELEV: the elevation of the stream bed at the upstream end of the current segment [L/T]
- WIDTH: the width of the stream at the upstream end of this segment [L]. This variable is used in the simulation for each stress period/segment with an <u>ICALC</u> =0. When ICALC is 1, the variable is read each stress period when <u>REACHINPUT</u> is active and <u>ISFROPT</u> is 0, and is only used for each segment in the first stress period in the simulation when REACHINPUT is active and ISFROPT is 4 or 5.
- **DEPTH**: the average depth of water in the channel at the upstream end of this segment [L]. This variable is only used in the simulation when <u>ICALC</u> =0. The stream

stage in a reach is assumed to equal the elevation of the top of the streambed (ELEV) plus the depth of water.

- **THTS**: the saturated water content (θ_s) in the unsaturated zone beneath the upstream end of the current segment [-]. This variable is read for the first stress period when <u>REACHINPUT</u> is active, <u>ICALC</u>=1 and <u>ISFROPT</u>=4 or 5.
- **THTI**: the initial water content (θ_i) beneath the upstream end of the current segment [-]. THTI must be less than or equal to THTS and greater than or equal to the THTS minus the specific yield defined in the associated model cells. This variable is read for the first stress period when <u>REACHINPUT</u> is active, <u>ICALC</u>=1 and <u>ISFROPT</u>=4 or 5.
- EPS: the Brooks-Corey exponent (ε) used in the relation between water content and hydraulic conductivity within the unsaturated zone beneath the upstream end of the current segment [-]. This variable is read for the first stress period when <u>REACHINPUT</u> is active, <u>ICALC</u>=1 and <u>ISFROPT</u>=4 or 5.
- UHC: the vertical saturated hydraulic conductivity of the unsaturated zone beneath the upstream end of the current segment [L/T]. This variable is necessary when using the BCF package, whereas it is optional when using LPF. This variable is read for the first stress period when <u>REACHINPUT</u> is active, <u>ICALC</u>=1 and <u>ISFROPT</u>=5.

Downstream Stream Segment Properties (Dataset 6c)

The following parameters are defined per stress period for the downstream end of <u>each</u> segment in the stream network:

- **HCOND**: the hydraulic conductivity of the bed at the downstream end of the current segment [L/T]
- THICKM: the thickness of the stream bed sediments at the downstream end of the current segment [L/T]
- ELEV: the elevation of the stream bed at the downstream end of the current segment [L/T]
- WIDTH: the width of the stream at the downstream end of this segment [L]. This variable is used in the simulation for each stress period/segment with an <u>ICALC</u> =0. When ICALC is 1, the variable is read each stress period when <u>REACHINPUT</u> is active and <u>ISFROPT</u> is 0, and is only used for each segment in the first stress period in the simulation when REACHINPUT is active and ISFROPT is 4 or 5.
- **DEPTH**: the average depth of water in the channel at the downstream end of this segment [L]. This variable is only used in the simulation when <u>ICALC</u> =0. The stream stage in a reach is assumed to equal the elevation of the top of the streambed (ELEV) plus the depth of water.
- THTS: the saturated water content (θ_s) in the unsaturated zone beneath the downstream end of the current segment [-]. This variable is read for the first stress period when <u>REACHINPUT</u> is active, <u>ICALC</u>=1 and <u>ISFROPT</u>=4 or 5.
- **THTI**: the initial water content (θ_i) beneath the downstream end of the current segment [-]. THTI must be less than or equal to THTS and greater than or equal to the THTS minus the specific yield defined in the associated model cells. This variable is read for the first stress period when <u>REACHINPUT</u> is active, <u>ICALC</u>=1 and <u>ISFROPT</u>=4 or 5.
- EPS: the Brooks-Corey exponent (ε) used in the relation between water content and hydraulic conductivity within the unsaturated zone beneath the downstream end of the current segment [-]. This variable is read for the first stress period when <u>REACHINPUT</u> is active, <u>ICALC</u>=1 and <u>ISFROPT</u>=4 or 5.

 UHC: the vertical saturated hydraulic conductivity of the unsaturated zone beneath the downstream end of the current segment [L/T]. This variable is necessary when using the BCF package, whereas it is optional when using LPF. This variable is read for the first stress period when <u>REACHINPUT</u> is active, <u>ICALC</u>=1 and <u>ISFROPT</u>=5.

Note that during the simulation, MODFLOW will linearly interpolate the upstream (dataset 6b) and downstream (downstream 6c) values to the midpoint of each reach.

Lake Properties

A brief summary of supported inputs for the Lakes tab is presented below:

😻 Surface water i	network	-		
•				
Name	Туре			
Surface Water Netwo	rk SFR2 ~			
Streams Lakes Ga	iges			
Index	Name			
1	East Lake			
2	West Lake			
		Realize lakes		
21-1				
2 lakes				
Assign to appropri	iate layer	Apply OK	Cano	cel

Static Lake Properties

The following parameters are defined per lake for the duration of the simulation period:

- Index: read-only unique integer identifier for each lake segment calculated by Visual MODFLOW Flex.
- **Name**: an optional text input name for the lake that can be used to label the segment in Flex viewers

Realize Lakes

Currently the main inputs for Lakes in the surface water workflow are the shapes of the lakes as well as the <u>topology</u>. More complex input data including the hydraulic properties and transient inputs for lakes are not currently supported in the Surface Water workflow. However, the "Realize lakes" button (shown above) allows you to convert each lake in the **Lakes1** layer to a separate LAK boundary condition that can be parametrized. For more information about LAK inputs, please see the <u>theory</u> section.

Stream and Lake Gage Properties

,				Editor Script							
Name Type Surface Water Network SFR2 ~				Gage Type Stag	e - ft	Station Type					
				$\frac{1}{\sqrt{x}}$ Calculation 1 \sqrt{x}						Reach 🗸	
trea	ms Lakes	Gages		Time	V	Value	V	Target Residual	7 ^	Stream:	
	Name 🛆		Station Type	•	31	159.7321661		1		Hungary Creek 🗸 🗸	
	vame ⊿ i	Host Feature	Station Type		60	142.8744266		1			
7					91	143.6874334		1			
•	Gage1	Hungary Creek			121	147.3343159		1		Stations: Show All	Add
	Gage2	Diversion	Reach		152	165.0154983		1		Gage1 ~	Delet
	Gage3	North Run	Reach		182	165.7849423		1			
	Gage4	L27	Lake		213	166.877402		1			
	-	L21			244	146.6333851		1		Downstream Position	
	Gage5	121	Lake		274	152.3049468		1		57.45 %	
					305	141.6419207		1			
					335	152.746161		1			
					366	158.466105		1			
					397	152.3505324		1			
					425	138.0797756		1			
					456	152.4580462		1			
					486	150.645025		1			
					517	145.5894033		1			
					547	143.06147		1	*		
				Load sched	ule object			✓ Load			
ga	jes										

A brief summary of supported inputs is presented below:

Static Gage Properties

The following parameters are defined per observation gage location for the duration of the simulation period:

- Name: an optional text input name for the gage that can be used to label the gage in Flex viewers and in the raw MODFLOW GAGE input file
- Host Feature: (read-only) name of the parent stream or lake feature on which the gage is located
- Station Type: (read-only) the type of station (i.e. Stream "Reach" or "Lake")

Gage Editor

The Gage Editor tab within the Surface Water Network Editor includes several controls allowing you to define and edit surface water observations. The Observation Schedule table and related controls in the middle of the window allows you to define the observations (e.g. time, value, and target residual) while the right side of the panel allows you to define the spatial scope over which the surface water observation(s) apply (e.g. the collection of cells where the volumetric flow is to be measured).

Observation Schedule

The left side of the Gage Editor dialog includes the following controls for all supported types of observations (boundary conditions, zone budget zones, stream, and lake gages):

 Gage Types: allows you to select the type of observation to be measured and associated project <u>units</u>. The stream and lake gages support a variety of observation types:

o Stream Reach gages:

- *Stage*: the elevation of the water surface at the midpoint of the observed reach
- *Outflow*: outflow from the stream reach
- Depth: the depth of the surface water feature at the midpoint of the observed reach
- *Width*: the width of flow at the midpoint of the reach
- *Midpoint Flow*: stream discharge at the midpoint of the observed reach
- Head Difference: head difference between stream midpoint and the associated groundwater cell centroid
- Gradient: groundwater gradient between the stream midpoint and the associated groundwater cell centroid
- Diverted Flow: the amount of flow diverted into the segment (upstream-most reach of diversion segments only),
- Pre-diversion Flow: the amount of flow discharge at the upstream junction of the diversion segment (upstream-most reach of diversion segments only)
- Groundwater Head: the head in the associated groundwater cell,
- Streambed Seepage: streambed seepage through the unsaturated zone (only available if ISFRRPT>2)
- Unsaturated Storage: storage in the unsaturated zone beneath the streambed (only available if ISFROPT>2)
- Recharge: amount of water reaching the water table from the stream bed seepage (only available if ISFROPT>2)
- <u>Lake gages</u>:
 - Stage: water surface elevation of the observed lake
 - Inflow: total inflows to the observed lake
 - Outflow: outflows from the observed lake
 - Uzf Runoff: runoff from the UZF package into the observed lake
 - Uzf Infiltration: flow from the observed lake to underlying unsaturated UZF zone cells
 - *Volume*: estimated volume of water in the observed lake
- **Toolbars:** the gage toolbars include the following buttons:
 - Add interval: adds an observation time at the end of the table
 - o 🖽 Insert interval after selection: adds an observation time after the selected row
 - Delete selected row(s): deletes selected row(s) from the table
 - Section 2012 or the sort order (if any) on fields in the observation table
 - $\circ \sqrt{x}$ Expression builder: opens the Expression builder
 - o III Assign to column: evaluates the Expression for all cells in the current column
 - Assign to current cell: evaluates the Expression for all selected cells in the current column (press and hold SHIFT or CTRL buttons with left mouse clicks to select multiple cells)
- Table: the table in the left hand side of Gage Editor includes three fields:

- o Time: elapsed time relative to the model start date
- o Value: the value of the observation
- Target Residual: the target difference between observed values and simulated results (based on measurement accuracy/variability, project goals, stakeholder input).
- Load Schedule Object: Selecting this option will allow you to load the data from a time schedule object in the Data Explorer and map fields from the schedule object (using the dropdown selectors) to the value and target residual fields.

Observation spatial scope

With the exception of certain stream and lake observations, the observation types apply generally apply over a defined area rather than at a discrete point. As such, the right side of the panel is used to define the spatial extent/scope of the observations that will be used for extracting simulated equivalent values to be compared to the observations. Since the various observation types have differing contexts, the applicable interface is dependent on the type of observation:

- Station Type: the type of gage: (stream) reach or lake
- Stream/Lake: the parent stream segment or lake feature where the observation is located
- **Stations**: the name of the current station. (Note: you can check the show all box to use the drop down to switch between gages).
- **Downstream Position**: allows you to place the observation along the length of the parent stream segment: 0 is the upstream end and 100 is the downstream end of the segment
- Add and Delete buttons: allow you to manage gages as described by the button label.

13 Expression Builder

The Expression Builder allows you to build and evaluate complex expressions on a variety of objects in Flex. The expressions can include basic arithmetic operations, mathematical functions, and distributed values from surfaces and horizons.

Scope

Expressions can be evaluated for the following objects in Visual MODFLOW Flex:

- Data Explorer Object Operations:
 - o Point, Polyline, and Polygon Elevations
 - o Surface Elevations
 - Map Elevations
 - o Edit Properties

• Model Explorer Objects

- Model Properties (Edit Properties Dialog)
- o Boundary Conditions (Edit Boundary Conditions Dialog)
- Surface Water (Edit Surface Water Network Dialog)

For Data Explorer Objects, the Expression Builder can be accessed by right-clicking on the object, selecting Settings... and clicking on the Operations node. For objects in the Model Explorer (like model properties and boundary condition objects), you can enter expressions directly in the Calculation toolbar (similar to what is shown in red below) or you can build

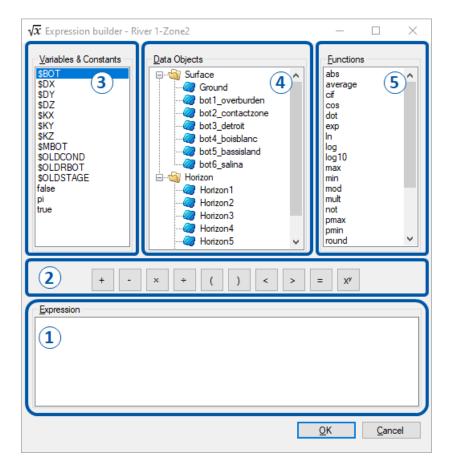
expressions with the assistance of the Expression Builder (\sqrt{x} button):

it Cells Script					_	
ones	Conductivity	🐍 Calculati	on	\sqrt{x} III III I		
Zone	Layer	▼ Row	▼ Column	√ Kx (m/s)	Ƴ Ky (m/s)	マ Kz (m/s) マ
1	▶ 1	1	1	0.0002	0.0002	0.0002
2	1	1	2	0.0002	0.0002	0.0002
	1	1	3	0.0002	0.0002	0.0002
	1	1	4	0.0002	0.0002	0.0002
	1	1	5	0.0002	0.0002	0.0002
	1	1	6	0.0002	0.0002	0.0002
	1	1	7	0.0002	0.0002	0.0002
	1	1	8	0.0002	0.0002	0.0002
	1	1	9	0.0002	0.0002	0.0002
	1	1	10	0.0002	0.0002	0.0002
	1	1	11	0.0002	0.0002	0.0002
	1	1	12	0.0002	0.0002	0.0002
	1	1	13	0.0002	0.0002	0.0002
	1	1	14	0.0002	0.0002	0.0002
	1	1	15	0.0002	0.0002	0.0002
	1	1	16	0.0002	0.0002	0.0002
	1	1	17	0.0002	0.0002	0.0002

Building Expressions

The Expression Builder can be used to construct mathematical expressions to specify variable property values (e.g. Kx, initial heads, Kd), boundary condition values (e.g. river conductance, constant head, etc.), or attribute values for shapes (e.g. points features in the Data Explorer). The Expression Builder is shown below for editing conductivity values. The Expression builder consists of five components:

- 1. Expression workspace: a workspace to build expressions;
- 2. <u>Operators</u>: basic arithmetic operators (e.g. addition, subtraction, multiplication, division, parentheses, and exponents);
- Variables & Constants: a list of variables associated with the current model cell and constants
- <u>Data Objects</u>: a list of supported data objects from the data explorer and model explorer windows
- 5. Functions: a list of supported mathematical, logical, and vector functions



Please Note: The expression builder is case sensitive.

Operators

The following operators are always available in the Expression Builder:

Operator	Butt on	Example	Result
Add	+	1+2	3
Subtract	-	4-3	1
Multiply	×	2*5	10
Divide	÷	2/4	0.5
Open bracket	(2*/5 · 2)	24
Close bracket)	3*(5+2)	21
Less Than	<	5<2	False
Greater Than	>	5>2	True
Equals	=	5=5	True
Power	Хх	5^3	125

Please Note: The expression builder does not support spaces between operators

Variables & Constants

The expression builder includes a list of applicable model properties or boundary condition values as well as standard constants as described below.

Grid Geometry Variables

The following grid-based variables are always available in the Expression Builder:

Variable	Description
\$BOT	cell bottom elevation
\$DX ¹	cell width in the x-direction
\$DY ¹	cell length in the y-direction
\$DZ	cell thickness

Variable	Description
\$MBOT	model bottom elevation
\$X	x-coordinate of grid cell centroid
\$Y	y-coordinate of grid cell centroid
Notes: ¹ - finite difference	e grids only

Editing Model Properties

The following variables are available in the Expression Builder during Model Property editing sessions:

Variable	Description
}	initial value of the specified field {fieldname} at the start of the edit session (e.g. \$OLDINITIALHEADS for the initial heads property field)

Assigning Boundary Conditions By Geometry

The following variables are available in the Expression Builder when assigning Boundary Conditions using polylines or polygons or using a (polyline or polygon) data object:

Variable	Description
\$FACEAREA_N ORTH	area of the current cell projected onto the model- coordinate XZ plane
\$FACEAREA_T OP	area of the current cell projected onto the XY plane (i.e. plan area)
\$FACEAREA_W EST	area of the current cell projected onto the model- coordinate YZ plane
\$RCHLNG ¹	length of the intersection between the current cell and the input polyline
\$LENGTH ¹	percentage along the length of the polyline from the beginning of the polyline to the exit point of the polyline from the current cell
\$SEGMENT ¹	ID of the polyline intersecting the cell
\$UCTOCOND	unit conversion factor for converting the length and time units used for hydraulic conductivity to the length and time units used for conductance
Notes: ¹ - polyline feature	es only

Editing Boundary Conditions

The following variables are available in the Expression Builder during Boundary Condition editing sessions:

Variable	Description
\$KX	horizontal conductivity along X-axis
\$KY	horizontal conductivity along Y-axis
\$KZ	vertical conductivity
\$MBOT	model bottom elevation
\$OLD{fieldname }	initial value of the specified field {fieldname} at the start of the edit session (e.g. \$OLDCOND for river conductance values)

Constants

The following constants are always available in the Expression Builder:

Keyword	Constant	Example	Result
false	False (constant)	false	0
pi	Pi (p) (constant)	pi cos(pi)	3.141592653 58979 -1
true	True (constant)	true	1

Data Objects

The Data Objects component of the Expression Builder includes a list of objects from the Data Explorer and the Model Explorer windows that can be included in expressions. Surfaces and horizons are currently supported. Values from the surface/horizon are bilinearly interpolated to the location of the cell centroid (in the case of finite difference grid and quadtree grids) and to the interior cell node (in the case of Voronoi grids). Note that bilinear interpolation is exptrapolated beyond the extents of a given surface.

The syntax to use a surface is *`object_name`* where *object_name* is the name of the surface in the Data Explorer or the name of the horizon in the Model Explorer, as applicable. Surfaces may be used in expressions:

Examples

• The expression \$`Ground`(\$X \$Y)-1 would result in a value of 1 unit of length below ground surface. This may be useful when defining features such as the bottom elevation of a river.

- The expression pmin(\$`Ground`(\$X \$Y) \$'Pit Elev'(\$X \$Y)) would result in the lower elevation between ground surface and a surface representing the elevation of an excavated pit.
- The expression ifgaps(\$`local`(\$X \$Y) \$`regional`(\$X \$Y)) compares local surface with a regional surface and uses the regional values where there are gaps in the local surface this is useful with two surfaces have differing extents

Functions

The following functions are always available in the Expression Builder:

Function	Descriptio n	Example	Result
abs	Absolute Value	abs(-1.2)	1.2
average	Average	average({1 2 3})	2
cif	Conditional If	cif(true 23 24) cif(false 23 24) cif(1 23 24) cif(0 23 24) cif(1-1 23 24)	23 24 23 24 24 24
cos	Cosine	cos(0)	1
dot	Dot Product	<pre>dot({1 2 3} {1 2 3})</pre>	14
equal	Equality	equal(2+2 4) equal(2+2 5) cif(equal(2+2 5) 23 24)	1 0 24
exp	Exponential	exp(1)	2.718281828 45905
ifgaps	Conditional If for noData values in a surface	ifgaps(surfA surfB)	returns surfA where it has valid values and surfB where it is absent or has noData values. surfA can be an expression

Function	Descriptio n	Example	Result
ln	Natural logarithm	ln(2.718218)	1
log	Logarithm	log(16 4)	2
log10	Base-10 logarithm	log10(100)	2
max	Maximum Value	<pre>max({10 2.2 34})</pre>	34
min	Minimum Value	min({10 2.2 34})	2.2
mod	Modulo	(10)mod(3)	1
mult	Multiplicatio n	<pre>mult({2.0 3.0 4.0})</pre>	24
not	Negation	<pre>not(true) not(false) not(1) not(0) not(2) not(1-1)</pre>	0 1 0 1 0 1
pmax	Maximum Value (pairwise)	pmax({10 2.2 34} {2 3 0.5})	{10 3 34}
pmin	Minimum Value (pairwise)	pmin({10 2.2 34} {2 3 0.5})	{2 2.2 0.5}
round	Round to Decimal Place	round(1.523 2) round(5.523 0)	1.52 10
sigdig	Round to significant digit	<pre>sigdig(1523 2) sigdig(1.523E+3 1)</pre>	1500 2000
sin	Sine	sin(pi/2)	1
sqrt	Square Root	sqrt(4)	2
sum	Sum	sum({1 2 3})	6
tan	Tangent	tan(pi/4)	1
vector	Vector	vector({3 2})	{2.0 2.0 2.0}
vequal	Vector Equality	<pre>vequal({1 2 3} {1 2 3}) cif(vequal({4 5</pre>	true 20
		6}	20

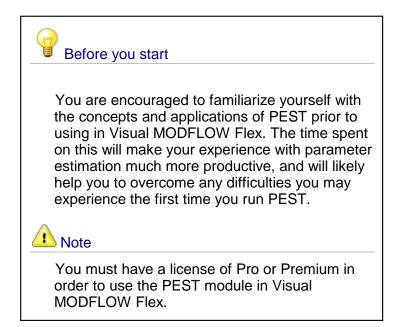
Function	Descriptio n	Example		Result
		6}) 10 20)	{4 6	

Examples are also provided in the help text, which you can view by hovering the mouse pointer over a given function. Note that surfaces and horizons are treated as vectors $\{ \}$ in the expressions.

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14 PEST (Parameter Estimation) Workflow

Visual MODFLOW Flex provides a seamless interface to the popular parameter estimation and predictive analysis program PEST, developed by Dr. John Doherty of Watermark Numerical Computing. This section provides instructions on using Visual MODFLOW Flex to setup, run, and interpret a Parameter Estimation/Predictive Analysis simulation. In addition, this chapter provides a brief description of the input parameters and settings required by PEST. A detailed description of the algorithms, parameters, input files, and other options for PEST are available in the PEST User Documentation. This can be accessed from www.PESTHomepage.org



Visual MODFLOW supports both the Calibration and Predictive Analysis capabilities of the PEST program, and it allows you to run parameter estimation using results from both groundwater flow and contaminant transport simulations (i.e. observations can consist of heads, concentrations, and groundwater flux). Support for transport, will be added in future releases.

Acknowledgements:

Excerpts from the following publications are used throughout this documentation:

- Using Pilot Points to Calibrate a MODFLOW/MT3D Model, Doherty (2008)
- PEST: Model-Independent Parameter Estimation, User Manual: 7th Edition, Doherty (2019)
- Addendum to the PEST Manual, June 2012
- <u>www.PESTHomepage.org</u>

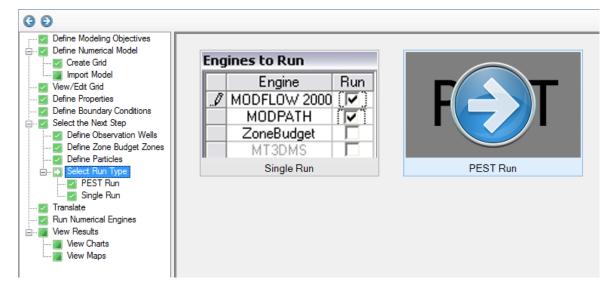
Suggested References:

Several USGS publications are also available on PEST. See:

- Approaches to Highly Parameterized Inversion: a Guide to Using PEST for Groundwater Model Calibration: <u>http://pubs.usgs.gov/sir/2010/5169/</u>
- Approaches to Highly Parameterized Inversion: a Guide to Using PEST for Model Parameter and Predictive Uncertainty Analysis" <u>http://pubs.usgs.gov/sir/2010/5211/</u>
- Approaches to Highly Parameterized Inversion: Pilot Point Theory, Guidelines and Research Directions <u>http://pubs.usgs.gov/sir/2010/5168/</u>

Loading the PEST Workflow

The PEST workflow can be launched from the "Select Run Type" step in a numerical workflow, as shown below; simply click on the PEST button in the main window.



Before attempting to run a parameter estimation simulation, make sure your model meets the following requirements:

- The model runs successfully (converges) and produces meaningful results. The model should provide a solution under a variety of input parameter conditions. Parameter estimation is as much an art as it is a science, and therefore, it should only be used to complement your own efforts in understanding the system.
- The model has one or more (preferably many more) observations against which to compare the calculated results. Observations can be in the form of measured or estimated values of head or concentration at discrete points in the model, or in the

form of measured or estimated groundwater fluxes into (or out of) one or more grid cells.

- It is also recommended that you do a sensitivity analysis prior to a full-fledged PEST run. In a sensitivity analysis, parameter values are individually changed to determine the effect on model calibration and prediction. The results give an indication of which parameter changes can have significant impact on the model results (these are sensitive parameters) and which parameter changes have little or no impact on the model results (these are non-sensitive or insensitive parameters). This should help you to property select parameters to include in a PEST run, as you should focus more on the sensitive parameters, and less on the non-sensitive parameters.
- The observation times (for heads) lie within the start/stop time of the numerical simulation. If you have imported a model from Visual MODFLOW Classic, ensure that an appropriate start date was defined in Visual MODFLOW Classic before loading the project into Visual MODFLOW Flex. If you have generated the numerical model from a conceptual model workflow, ensure that the start date at the modeling objectives is appropriate based on the head observation times you have defined.

Setting up a PEST Run

PEST requires several inputs and a number of steps that must be completed in a specific order. Fortunately, Visual MODFLOW Flex provides the PEST GUI in a workflow, that guides you through the sequential steps and necessary inputs, running PEST, and analyzing the results:

- Define Observations and Assign Weights
- Define Parameters (Property Zones, Boundary Conditions)
- Define Pilot Points
- Define Kriging Variograms
- Select Regularization (None, Tikhonov, SVD Assist)
- Define <u>PEST Run Settings</u> and Run PEST
- <u>Run Sensitivity Analysis</u>
- Analyze Results
- Update Model Inputs

14.1 Define Observations

When PEST is used to assist in the calibration of a model, it is tasked with minimizing an objective function, represented by the symbol F. This is comprised of the sum of the weighted squared deviations between the calculated (X_{calc}) and observed (X_{obs}) system responses and is ultimately a function of the <u>defined Parameters</u> (p_j). The difference between the calculated and observed values are referred to as a residual, and represented by the following equation:

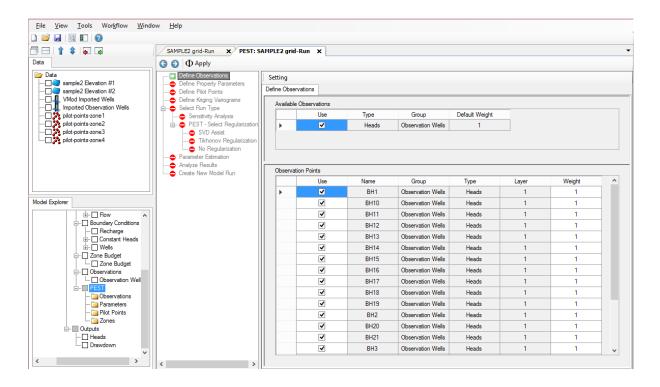
$$r_i = X_{calc} - X_{calc}$$

In the simplest PEST run, the objective function (F) is calculated using the following equation:

$$\Phi = \sum_{i}^{n} min(r_i) = f\left(p_j\right)$$

In the case of a groundwater model, these system responses are typically head at a point in space, concentration at a point in space, or groundwater flow to a specified zone.

At the Define Observations step, you will see a list of all your available head observations as shown in the following figure:



The observation values are assigned a default weight of 1.0, which means the residual will not be modified, and all observations will be treated equally.

We want PEST to:

- give more weight to measurements that you can trust
- give greater priority to measurements in areas where predictions are important
- decrease bias that is introduced by denser data (if appropriate)
- give equal weight to observations with different units (eg. Heads vs. Fluxes, vs Concentrations)

The weight factor is commonly used to normalize observations of different types. For example, when you have head and flux observations included in the same PEST run, the flux residuals are typically much higher than a head residual. For example:

- a flux residual for a set of cells could be +/- 1000 m3/day
- a head residual at a single cell is +/- 1m.

PEST calculates the objective function by summing the squares of these residuals, which results in flux observation residuals being several orders of magnitude greater than the head residuals. As a result, PEST will focus more on minimizing the flux residuals, and less so on the head residuals, which is most likely undesired from the modeler's view point.

The solution is a user-defined weighting factor (w_i)

$$\Phi = \sum_{i}^{n} min(w_{i}r_{i})$$

We use a weight less than 1.0 to reduce the magnitude of flux errors so they are comparable to head errors. A similar problem is often seen with concentration targets, for the same reason. The ability to use weights to address a variety of common calibration issues makes the objective more useful.

Settings

If you click on the [Setting] button above the Observations grid, you can adjust the Time Extrapolation Limit; this value is used by PEST to search for the nearest observation time for comparing to calculated MODFLOW output times. The higher the value, the more likelihood that an observation time can be found to match the MODFLOW output times. The default is 100 (in the project time units).

Please Note: the value of the Time Extrapolation Limit is particularly important for matching observations with Steady State models as the time for comparison is the steady state simulation period. If you have a particularly short (e.g. 1 day) or long (e.g. 10 year) steady state simulation period, your PEST analysis may not have any valid observations (or fewer than expected), depending on the model start date relative to the date(s) of the observations.

14.2 Define Parameters

At the Define PEST Parameters step, select which model input types you wish to include in the PEST run.

e Observations e Property Parameters	Define Prop	erty Parameters						
ne Pilot Points	Select P	arameter:						
 Define Kriging Variograms Select Run Type 		Use	Group	Parameter	Tied To	Transform	ation	
sitivity Analysis	▶	✓	Conductivity	Kx	None	- Log	-	
T - Select Regularization			Conductivity	Kz	None	- Log	•	
SVD Assist Tikhonov Regularization			Storage	Ss	None	 None 	•	
No Regularization eter Estimation e Results New Model Run		roperty Zone:	Storage	Sy	None	None	-	
No Regularization er Estimation Results			Storage	Sy Zone	Value	Min	•	Max
Regularization Estimation sults		roperty Zone:		· · · · · · · · · · · · · · · · · · ·			•	
Regularization Estimation sults		roperty Zone:	Parameter	Zone	Value		•	300
Regularization Estimation esults		roperty Zone: Use	Parameter Kx	Zone 1	Value 30	Min		Max 300 300 300

Parameter Settings

In the table at the top of the window, select which parameter(s) you want to include; Visual MODFLOW Flex currently supports the following parameters:

- Conductivity (Kx and Kz)
- Storage (Ss and Sy)

Please Note: Ss and Sy should only be included in a transient MODFLOW run

This list of available parameters will be extended in future versions to include more parameters from both the flow and transport models.

Select the check-box in the Use column in order to include this parameter zone.

Tied To

• **Tied**: The parameter value is tied (linked) to the value of another parameter, in which case this parameter takes only a limited role in the parameter estimation process. If you select the tied to option, then you can select the parent parameter from the dropdown list.

Please Note: you can only tie to other parameters that have been
selected/included in the PEST run). PEST does not allow a parameter to be tied to a
fixed parameter, or a parameter that is already tied to another parameter.

If a parameter is tied to a parent parameter, the parameter "piggy-backs" on the parent parameter during the estimation process. In this way, the ratio between the initial values of the parameter and its parent remain constant throughout the estimation process.

Transformation

In many cases, the linearity assumption on which PEST is based is more valid when certain parameters are log-transformed. This means that the log-transformation of some parameters can often make the difference between success and failure of the estimation process. However, a parameter that can become zero or negative during the estimation process must not be log-transformed.

The parameter Transformation field controls how the parameter value will be transformed during the optimization process. There are three transformation options:

- Fixed: The parameter value is fixed and takes no part in the parameter estimation process.
- Log: The parameter will be log-transformed (i.e. the log value of the parameter is optimized rather than the 'real' value of the parameter).
- None: No transformation takes place (i.e. the 'real' parameter value is adjusted)

If the parameter is log-transformed then the covariance, correlation coefficients and eigenvector values refer to the log of the parameter. However, the parameter estimates and confidence intervals refer to the untransformed parameter.

If you fix a parameter, its value will be fixed at its initial value, and it will not be part of the estimation process.

Parameter Zone Settings

In the table at the bottom of the window, select which parameter zones you wish to include; by default, all zones from a selected parameter type will be included. The Value column indicates the value for each zone; in the case where you have distributed parameter values in a zone, you will see "Distributed" in this column. The Minimum and Maximum are the lower and upper bounds of the parameter zone.

The lower and upper bounds should be chosen wisely; for example, if you know that a zone represents an sandy-gravel aquifer, then define practical limits for the upper and lower bounds for conductivity for sandy-gravel. The default values are 1E-15 and 1E+30 respectively. The lower and upper bounds are ignored for fixed and tied parameters. If an updated parameter value is outside of its bounds, PEST temporarily holds the parameter at its boundary value.

Updating Parameter Values after a PEST Run

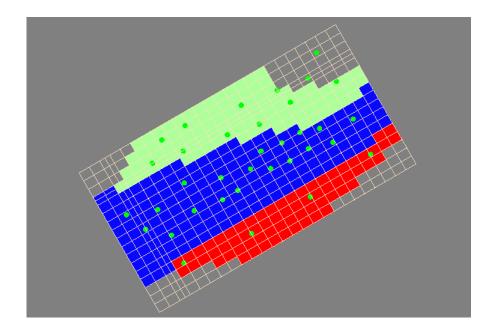
If you have completed a PEST run and return to the Define Parameters step to make a change (such as add/remove zones or adjust the Minimum or Maximum values), you need to click the [Apply] button on the workflow toolbar, and also proceed through the <u>Define Pilot</u> <u>Points</u> step, and re-generate the <u>Define Kriging Variograms</u> step in order to update the appropriate input files.

14.3 Define Pilot Points

The next step is to define Pilot Points.

SAMPLE2 grid-Run × PEST: SAMPI	LE2 grid-Run X								•
🔇 🜔 Ф Аррly									
	fine Pilot Points								
Define Property Parameters Define Pilot Points Define Kiging Variograms Select Run Type	Pilot Points				Parameter	7			
Sensitivity Analysis	Pilot Points Name		Group		Varameter / Used	Zones Parame	ter Zor		
SVD Assist	pilot-points-zone1		pilot-points-zone1			Kx	1		
Tikhonov Regularization	pilot-points-zone2		pilot-points-zone2				'		
Parameter Estimation	pilot-points-zone3		pilot-points-zone3			Kx	2		
Analyze Results	pilot-points-zone4		pilot-points-zone4			Kx	3		
			pilot pointo cono r		~	Кх	4		
`									
	Parameter Zone Sel	ection							
	Kx_Zone4		*						
	Used	Fixed	Name	Group	Х		Y	Value	
	▶ ✓		pp0	pilot-points-zone4	44718.53	66 7	763280.9756	30	

Pilot points are simple XY points with an initial value for each parameter that you want PEST to estimate. Pilot points can be imported from .TXT file, XLS, .SHP file, or assigned manually by digitizing in the 2D environment. An example of the pilot points on top of conductivity zones is shown below.



The general steps are as follows:

- Select the desired points object from the model tree
- Click (Next Step button) to add these points.
- Select which parameter zones the points represents (eg. Kx-Zone1, or Kz-Zone5)

In the table in the lower half of the window, specify which pilot points are "Fixed". Fixed pilot points are those that have initial values that are well known, and will not be adjusted during the PEST run. Examples of these include points where you have pumping/slug test data. For all other points, their initial value is taken from the property zone in which the specific point lies.

Visual MODFLOW Flex handles these "Fixed" pilot points the following way: In the PEST Control file,

- these pilot points parameters use "Fixed" Transformation, and the initial value defined in the table above will appear beside each point; and
- the regularization information for these fixed parameters is not included under the *prior information section. This is only applicable when one of the regularization options are used in the PEST run.

Once you are finished, be sure to repeat these steps for the other parameter zones you have included.



You must create a distinct set of pilot points for each of the parameter-zones you selected in the previous step.

Theory

Using conventional model calibration technology, the calibration process would use one parameter associated with a property zone, and adjusting these parameters until the fit between model outcomes and field observations is as good as possible. If the goodness of fit obtained on the basis of these zones was not acceptable, then extra zones would be introduced into the model domain at locations where the modeler felt that they would "do the most good"; the parameterization process would then be repeated with the new parameters included. If a good fit was still not obtained, more zones would then be introduced. The process would continue until the fit between model outcomes and field observations was acceptable.

There are a number of shortcomings associated with this approach. These include the following:

- The procedure is quite laborious and slow.
- In a case such as the present one, geological mapping provides no guidance on where to put extra zones; hence the final distribution of zones that the modeler achieves using this process is likely to be subjective and non-unique.
- Characterization of geological heterogeneity in the present study area by zones of piecewise uniformity is not in harmony with the nature of the alluvial material; therefore any zonation pattern that is finally decided upon will not "look right"; it will be defensible only on the basis that it is better to employ such a zonation scheme than to ignore geological heterogeneity altogether.
- Piecewise constancy as a method of characterizing geological heterogeneity lacks the flexibility required to explore the effects of small scale geological variability on model predictive uncertainty.

To overcome these problems, the distribution of transmissivity within the model domain will be described by a set of pilot points. A number of these pilot points will be introduced to the model domain and PEST will be asked to estimate the transmissivity of the aquifer at each such point. These "point-transmissivities" will then be spatially interpolated to all of the active cells within the model domain using Kriging. Hence in estimating transmissivity values at pilot points, PEST will effectively be assigning parameter values to the whole of the model domain.

Individual pilot points can be assigned to different zones within the model domain. Only those points assigned to a particular zone can be used in calculating transmissivity values throughout that zone using the Kriging interpolation procedure. Furthermore, the variogram upon which Kriging is based can be different in each zone, reflecting differences in the geology, or in the level of heterogeneity, expected within each geological unit. Note that if

only one pilot point is assigned to a particular zone, then that zone is characterised as being uniform.

Conventional wisdom dictates that the number of parameters involved in a parameter estimation exercise should be kept to a minimum. However when using pilot points in conjunction with PEST's new regularization mode, the opposite is often true. PEST's regularization functionality prevents the onset of numerical instability which often accompanies attempts to solve over-parameterised inverse problems. Furthermore, a superfluity of pilot points allows PEST to achieve a much better fit between model outcomes and field observations.

Reference: Calibration and Uncertainty Analysis for Complex Environmental Models, by John Doherty (2015).

General Tips

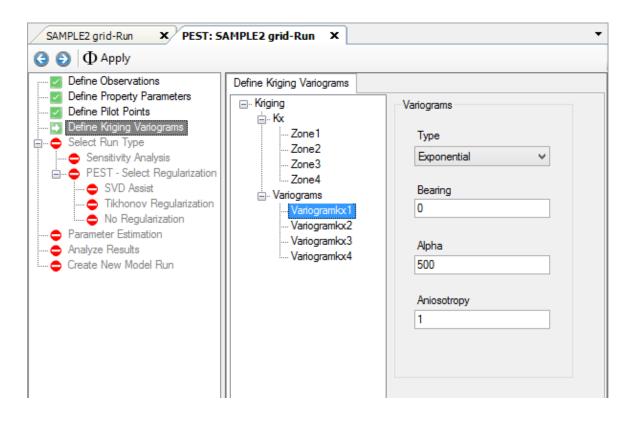
General tips on using pilots points (excerpted from http://www.pesthomepage.org/PEST_FAQ.php)

- There is no need to be parsimonious; use as many pilot points as you can. Let PEST do the regularization (use SVD, Tikhonov, SVD-assist or all of these together).
- Use more pilot points in those parts of the model domain where information has a high spatial density (for example where there are more observation wells).
- Try to place pilot points between head measurement wells in the direction of groundwater flow where they represent hydraulic conductivity. Place them on measurement wells where they represent specific yield or storage coefficient.
- Make sure you place hydraulic conductivity pilot points between measurement wells and any downstream boundary, for it is the hydraulic conductivity of the material between these wells and the boundary that determines the heads in those wells.
- Don't leave any large gaps in the final pilot points pattern.
- If you use preferred value regularization (i.e. you have selected Preferred Value <u>Tikhonov Regularization</u>) consider using a covariance matrix instead of weights for the prior information equations. See the PPCOV utility from the Groundwater Data Utilities suite.
- If you are absolutely sure that no heterogeneity can arise over a distance of less than x, then don't place any pilot points closer together than a distance of x.

14.4 Define Kriging Variograms

Once the pilot points are generated, the next step is to specify the Kriging settings that will be used to interpolate the pilot point data during PEST calibrations for these zones. Principally, this involves definition of the appropriate variogram. Variograms are also used

by PEST in the calculation of regularization weights and so are an important part of the process.



Visual MODFLOW Flex will create one default variogram for each parameter zone "structure".

Visual MODFLOW Flex uses Ordinary Kriging to interpolate between pilot points. This method has the following advantages:

- numerically efficient
- respects values assigned to the points
- regularization and interpolation can be based on same variogram

The only downside is that it requires a defined variogram to be effective and each parameter+zone must have its own variogram.

In Visual MODFLOW Flex, a default variogram is provided for each parameter+zone. Suggested defaults are:

- Exponential Variogram Type
- A = approx 20% of the length or width (whichever is greater) of the model domain; typical range is 20-70%
- Anisotropy = 1 (uniform)
- Nugget = 0

Select the desired Parameter zone from the tree, and provide the necessary variogram parameters.

 Please Note: Gaussian variograms are not recommended for use with PEST because they can lead to spurious interpolated property fields greater than or less than the highest/lowest property value assigned to any pilot point (Doherty, 2008a).

 Define Observations Define Property Parameters Define Pilot Points Define Kiging Vanograms Select Run Type No Regularization No Regularization Parameter Estimation Analyze Results Create New Model Run 	Define Kriging Variograms	Structure Nugget 0 Transform log Number of Variograms 1 Weight 0.15 Kriging Min. Number of Points 1 Max. Number of Points 50 Search Radius 2000
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Theory

Spatial Interpolation using Pilot Points

The use of pilot points in characterizing the spatial distribution of a hydraulic property must be accompanied by a mechanism whereby hydraulic property values assigned to pilot points are spatially interpolated to the cells of the finite difference grid. Spatial interpolation is accomplished using the Kriging algorithm. Kriging is a method of spatial interpolation based on geostatistics. The cornerstone of geostatistics is the variogram; a variogram describes the extent to which hydraulic property values (or any other type of data) pertaining to any two points are likely to be different from each other as a function of the distance between those points. One of the benefits of using Kriging as a basis for spatial interpolation is that the factors by which hydraulic properties at pilot points are multiplied before summation to obtain the hydraulic property value at a particular grid cell are independent of the actual hydraulic property values at the pilot points. Hence a set of "Kriging factors" pertaining to each of the cells of the finite difference grid can be calculated in advance of the actual interpolation process. As the latter is undertaken again and again as the model is run repeatedly by PEST, the fact that it is not necessary to repeat calculation of the Kriging factors on each occasion that the model is run can result in large savings in the time required to complete the overall parameter estimation process.

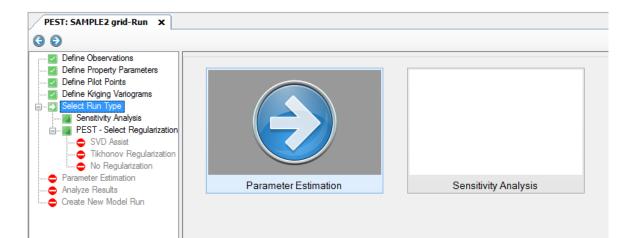
Calculation of Kriging factors is undertaken by program PPK2FAC. Variograms upon which these Kriging factors are based are supplied to PPK2FAC in a "structure file". Such a file is struct.dat. Inspect this file using your screen editor. For full details of the specifications of this file, see the documentation to the Groundwater Data Utilities. Note that the variogram assigned to zones that have just a single pilot point is quite unimportant; because there is only one pilot point assigned to each of them, all cells within these zones will be assigned the one interpolated value (same as the respective pilot point) irrespective of the variogram.

Also note that for all of the structures appearing in file struct.dat, the TRANSFORM variable is set to "log". Thus any variogram cited in each of these structures must pertain to the spatial distribution of the logarithm of the pertinent hydraulic property. This is in accord with the fact that most studies cited in the groundwater literature which treat transmissivity and/or hydraulic conductivity as a regionalized variable indicate that its distribution is better described by a log variogram than by a variogram based on native property values.

14.5 Select Run Type

At this step, you can select one of two types of PEST run:

- <u>Run Parameter Estimation</u> for finding the optimal set of parameters, based on your observations
- <u>Run Sensitivity Analysis</u> to calculate parameter sensitivities, which will help you to determine which parameters are influential or not-influential on the model results (based on the current values of the parameters).

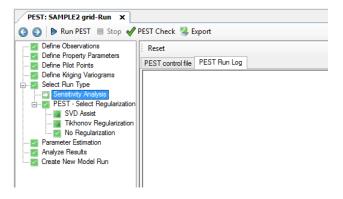


14.5.1 Run Sensitivity Analysis

A sensitivity analysis is the first step in assessing the possible range of results that can be derived from the groundwater model.

In a sensitivity analysis, parameter values are individually changed to determine the effect on model calibration and prediction. The results give an indication of which parameter changes can have significant impact on the model results (these are sensitive parameters) and which parameter changes have little or no impact on the model results (these are non-sensitive or insensitive parameters). This should help you to properly select parameters to include in a PEST run, as you should focus more on the sensitive parameters, and less on the non-sensitive parameters.

When you go to Run Sensitivity Analysis, the following window will appear:



Under the "PEST Control file" tab, you can see the PEST control file has been automatically generated for you with the appropriate settings for a Sensitivity Run.

PEST: SAMPLE2 grid-Run X	
🕒 🕑 🕨 Run PEST 🔲 Stop 🖋	PEST Check 🥞 Export
 Define Observations Define Property Parameters Define Pilot Points Select Run Type PEST - Select Regularization SVD Assist No Regularization Parameter Estimation Analyze Results Create New Model Run 	Reset PEST control file PEST Run Log pcf * * control data restart regularisation 35 21 4 412 2 1 1 1 single point 1 0 0 5.0 2.0 0.3 0.01 1 5.0 5.0 0.001 0.1 0.1 0.005 4 3 0.01 3 111 * parameter groups pg1 relative 0.01 0.0 switch 1.5 parabolic pg2 relative 0.01 0.0 switch 1.5 parabolic pg3 relative 0.01 0.0 switch 1.5 parabolic pg3 relative 0.01 0.0 switch 1.5 parabolic pg4 relative 0.01 0.0 switch 1.5 parabolic pg4 relative 0.01 0.0 switch 1.5 parabolic pg4 relative 0.01 0.0 switch 1.5 parabolic pg4 relative 0.01 0.0 switch 1.5 parabolic pg4 relative 0.01 0.0 switch 1.5 parabolic pg4 relative 0.01 0.0 switch 1.5 parabolic pg4 relative 0.01 0.0 switch 1.5 parabolic pg4 relative 0.01 0.0 switch 1.5 parabolic pg4 relative 0.01 0.0 switch 1.5 parabolic pg1-1 log factor 30 1 300 pg1 1.0 0.0 1 pg1-3 log factor 30 1 300 pg1 1.0 0.0 1 pg1-3 log factor 30 1 300 pg1 1.0 0.0 1 pg1-8 log factor 30 1 300 pg1 1.0 0.0 1 pg1-8 log factor 30 1 300 pg1 1.0 0.0 1 pg1-11 log factor 30 1 300 pg1 1.0 0.0 1 pg1-12 log factor 30 1 300 pg1 1.0 0.0 1 pg1-13 log factor 30 1 300

Run PEST

Click on to start the PEST Run; you should see the PEST progress in a DOS window.

When the run completes, you will see several new tabs added to the workflow window.

Define Observations	Reset					
Oefine Property Parameters Oefine Pilot Points	PEST control file	PEST Run Log	pest_jac.rec	pest_jac.sen	pest_jac.seo	pest_jac.res
Define Kriging Variograms Select Run Type Senstivity Analysis PEST - Select Regularization SVD Assist Tikhonov Regularisation No Regularization Analyze Results Update Model Inputs	pcf "control data restart regularisatio 35 21 4 412 2 11 single point 10 5.0 5.0 0.001 0.1 1.0005 4 3 0.013 11 11 "parameter groupp pg1 relative 0.010 pg2 relative 0.010 pg4 relative 0.010 pg4 relative 0.010 gg1-2 log factor 33 pg1-3 log factor 33 pg1-3 log factor 33 pg1-5 log factor 33 pg1-5 log factor 33 pg1-5 log factor 33 pg1-5 log factor 33 pg1-9 log factor 34 pg1-9 log factor 3	5 5.0 switch 1.5 para 0.0 switch 1.5 para 0.0 switch 1.5 para 0.0 switch 1.5 para 0.1 300 pg1 1.0 0. 0 1 300 pg1 1.0 0.	bolic bolic bolic 0 1 0 1 0 1 0 1 0 1 0 1 0 1 0 1 0 1 0 1			

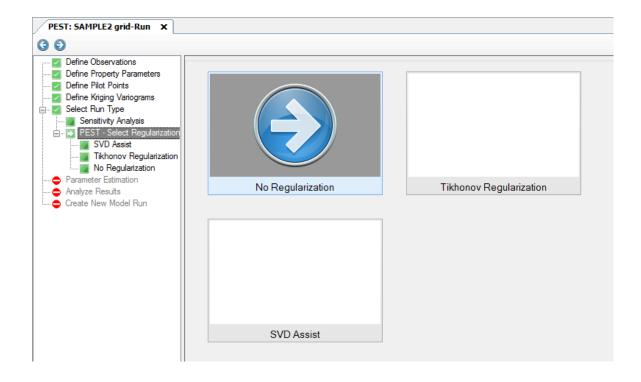
- Record file (.REC)
- Sensitivities for Observations Composite Sensitivities (.SEO)
- Sensitivities for Parameters (.SEN)
- Residuals (.RES)

Select the appropriate tab and you will see the sensitivities for the parameters and observations, along with other useful PEST run results.

14.5.2 Select Regularization

At this step, choose which regularization options you want to use in the PEST Run.

- No Regularization
- Tikhonov Regularization
- SVD Assist



Theory

One of the great advantages of using pilot points is that we can distribute a superfluity of those points throughout the model domain and then ask PEST to find for itself those regions within the study area where transmissivity must be greater or less than average in order to ensure that there is good agreement between model outputs and field measurements. If we had based our parameterization of the model domain solely on zones, we might not have placed those zones in the correct position for the calibration process to properly infer the existence or extent of such heterogeneity.

The introduction of regularization into the calibration process serves two purposes. Firstly it brings a high degree of numerical stability to a parameter estimation problem which would otherwise be highly susceptible to the deleterious effects of a singular normal matrix (you might have noticed when inspecting hcal.rec that PEST was not able to calculate any parameter statistics due to singularity of the normal matrix.) Secondly, if regularization constraints are appropriately defined, model calibration can proceed with a "homogeneous unless proven otherwise" philosophy; that is, in spite of the number of parameters at its disposal, PEST will make each zone within the model domain as uniform as it can in terms of the distribution of the estimated hydraulic property, introducing heterogeneity into a zone only where this is necessary in order to allow a good of fit between model outputs and field data to be achieved. Hence any heterogeneity which is introduced as an outcome of the calibration process is "there because it has to be there". In many modeling contexts this philosophy of model calibration has a large intuitive appeal, allowing a modeler to use zones to characterize the distribution of some hydraulic property within a model domain while, at the same time, removing the inflexibility that accompanies the characterization of a model domain by areas of piecewise parameter constancy.

Relationships between pairs of parameter values can be introduced into the calibration process as prior information equations. The weight assigned to each of these prior

information equations can be the same. Alternatively, if the weight is proportional to the inverse of the square root of the variogram calculated for the distance between the respective pilot points, then it can be shown that this is in harmony with the geostatistical characterization of the area as encapsulated in the variogram. What this characterization says, in short, is that "the closer are two points together, the more likely are the hydraulic properties at those points to be the same". By calculating weights on the basis of the inverse of the variogram, we are enforcing the "zero difference" condition more strongly for points which are closer together than for those which are farther apart.

When run in this mode, a number of control variables are required in the PEST control file, in addition to those required when PEST is run in "parameter estimation" mode. One of these variables is PHIMLIM. This specifies the degree of model-to-measurement misfit that is allowed to occur in the present optimization process. Because the attainment of a good model-to-measurement fit, and the simultaneous enforcement of homogeneity constraints, may place conflicting requirements on parameter values, a compromise between the two must be reached. The user determines the "compromise level" by setting a maximum model-to-measurement misfit that he/she will tolerate, this misfit being expressed in terms of the "measurement objective function". The maximum permissible value of the measurement objective function (ie. PHIMLIM) should be set a little higher than the objective function than it is possible to achieve without any regularization constraints being enforced.

Each prior information equation included in the parameter estimation process must be assigned a weight. As was discussed above, weights are calculated on the basis of geostatistical information available (or assumed) for the model area. If an observation or prior information equation is used for regularization purposes, then it is assigned to the observation group "regul". As part of its regularization functionality, PEST adjusts the weights assigned to all members of this group during each iteration of the optimization process; however the relative weight values within this group remain the same. The "regularization weight factor" by which the initial weights of all members of the group "regul" are multiplied during each optimization iteration is calculated in such a way as to respect the PHIMLIM value provided by the user as the maximum tolerable model-to-measurement misfit for the current case. An initial regularization weight factor needs to be supplied by the user.

14.5.2.1 No Regularization

If you choose the No Regularization option, then no further settings need to be adjusted prior to the PEST run. You will be presented with the PEST Control file, whereby you can edit/adjust values such as the PEST objective function goal, number of iterations, etc. Please consult the PEST users manual for an explanation of these parameters.

PEST: SAMPLE2 grid-Run X	
🕒 🕑 🖌 PEST Check	
 Define Observations Define Property Parameters Define Pilot Points Define Kriging Variograms Select Run Type Sensitivity Analysis PEST - Select Regularization SVD Assist Tikhonov Regularization No Regularization Analyze Results Create New Model Run 	Reset PEST control file pcf * control data restart estimation 35 21 4 0 1 1 1 single point 1 0 0 5.0 5.0 0.001 0.1 25 0.005 4 3 0.01 3 11 1 * parameter groups pg1 relative 0.01 0.0 switch 1.5 parabolic pg2 relative 0.01 0.0 switch 1.5 parabolic pg3 relative 0.01 0.0 switch 1.5 parabolic pg3 relative 0.01 0.0 switch 1.5 parabolic pg3 relative 0.01 0.0 switch 1.5 parabolic pg4 relative 0.01 0.0 switch 1.5 parabolic pg3 relative 0.01 0.0 switch 1.5 parabolic pg4 relative 0.01 0.0 switch 1.5 parabolic pg3 relative 0.01 0.0 switch 1.5 parabolic pg4 relative 0.01 0.0 switch 1.5 parabolic pg1 relati

14.5.2.2 Tikhonov Regularization

When you select Tikhonov Regularization, the PEST control file will automatically be generated to support this feature.

Select the [Generate Tikhonov Regularization] button to select the type of regularization.

- **Preferred Homogenous (Smoothness)**: Prior information equations relate the pilot points to one another. Pilot points that are near one another should have close values; only enough heterogeneity will be introduced to the system as necessary, the level of the heterogeneity being controlled by the pertaining semi-variogram.
- **Preferred Value**: Prior information equations relate the pilot points to their initial value. PEST will try to find a value that is as close to the initial pilot point value as possible.

PEST: SAMPLE2 grid-Run × () () () () () () ()	
 Define Observations Define Property Parameters Define Pilot Points Define Kiging Variograms Select Run Type Select Run Type Sensitivity Analysis SYD Assist No Regularization Parameter Estimation Analyze Results Create New Model Run 	Generate Tikhonov Regularization PEST control file pcf * control data restart regularisation 35 21 35 21 4 412 1 1 single point 10 5.0 2.0 5.0 2.0 7 5.0

When you are finished, proceed to the [Run PEST] step to begin the PEST run.

14.5.2.3 SVD Assist

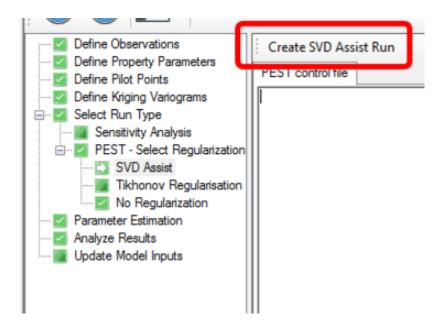
Theory

In contrast to Tikhonov regularization, which adds information to the calibration process in order to achieve numerical stability, subspace methods achieve numerical stability through subtracting parameters, and/or parameter combinations, from the calibration process (Aster and others, 2005). As a result of the subtraction, the calibration process is no longer required to estimate either individual parameters or combinations of correlated parameters that are inestimable on the basis of the calibration dataset. These combinations are automatically determined through singular value decomposition (SVD) of the weighted Jacobian matrix (Doherty and Hunt, 2010).

When PEST implements "SVD-assisted" parameter estimation, it computes the global Jacobian matrix only once. Then it decomposes parameter space into estimable and inestimable parameter combinations. It then reformulates the whole calibration problem so that, from that moment on, it estimates only "super parameters". Only as many of these are required as there are dimensions in the calibration solution space; alternatively, only as many of these need to be defined as you have computing resources to estimate. Through the use of super parameters you can get all of the benefits of highly parameterized inversion

with a comparatively small run time burden. Your model can have hundreds, or even thousands, of parameters, but these may be accommodated with a computational burden of only a few tens of runs per iteration.

Click on the [Create SVD Assist Run] button on the toolbar, as shown below.



The following Settings dialog will appear. For SVD Assist, you must provide the number of Super Parameters to use. Please consult the PEST manual for a recommended set of parameter values.

1066	Visual MODFLOW Flex 9.0 Help

Number of Super	r Parameters:
4	
Number of Optim	ization Iterations:
25	
Upper level of m	odel-to-measurement misfit (PHIMLIM)
20	
Acceptable level	of measurement objective function (PHIMACCEPT)
21	
	OK Cancel
	Chi Canoci

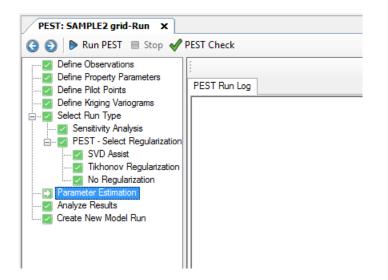
After clicking OK in the settings window, the PEST Control file, customized for an SVD Assist run, will be populated as shown below.

Define Observations	Create SVD Assist Run
	DEGT - LA
	PEST control file
	pcf
Select Run Type	* control data
Sensitivity Analysis	restart regularisation
	10 433 1 0 2
PEST - Select Regularization	1 2 double point 1 0 0
SVD Assist	5.0 2.0 0.3 0.03 10
📓 Tikhonov Regularisation	0.1 10.0 0.001
No Regularization	0.1 25 0.005 4 4 0.005 4
Parameter Estimation	25 0.005 4 4 0.005 4 1 1 1
Analyze Results	svd assist
Update Model Inputs	pest jac.pst
in poare model inputs	pest jac.joc
	0201
	* parameter groups
	pargp absolute 0.015 0.0 switch 2.0 parabolic
	* parameter data
	par1 none relative 10 1E-20 1E+20 pargp 1.0 -10.0 1
	par2 none relative 10 1E-20 1E+20 pargp 1.0 -10.0 1
	par3 none relative 10 1E-20 1E+20 pargp 1.0 -10.0 1
	par4 none relative 10 1E-20 1E+20 pargp 1.0 -10.0 1
	par5 none relative 10 1E-20 1E+20 pargp 1.0 -10.0 1
	par6 none relative 10 1E-20 1E+20 pargp 1.0 -10.0 1 par7 none relative 10 1E-20 1E+20 pargp 1.0 -10.0 1
	pars none relative 10 1E-20 1E+20 pargp 1.0 -10.0 1
	par9 none relative 10 1E-20 1E+20 pargp 1.0 -10.0 1
	par10 none relative 10 1E-20 1E+20 pargp 1.0 -10.0 1
	* observation groups
	regul1
	og000001
	* observation data
	OH11-09-20160000001 22.78002 1.0 og000001
	OH11-09-20160000002 21.0 1.0 og000001
	OH11-09-201600000003 21.19999 1.0 og000001
	OH11-09-201600000004 26.49999 1.0 og000001 OH11-09-201600000005 25.75998 1.0 og000001
	OH11-09-20160000006 26.04997 1.0 og000001
	OH11-09-201600000007 27.05997 1.0 og000001
	OH11-09-20160000008 28.00996 1.0 og000001
	OH11-09-201600000009 27.59996 1.0 og000001
	OH11-09-201600000010 21.43995 1.0 og000001
	OH11-09-201600000011 20.92994 1.0 og0000001

When you are finished, proceed to the [Run PEST] step to begin the PEST run.

14.6 Run PEST

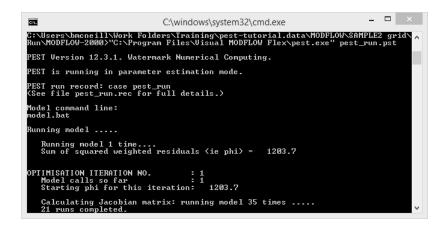
At this step, you can run PEST Check and start/stop the PEST run.



Before launching the PEST run, it is a good idea to run PEST Check. This PEST utility will check all the input files to ensure they meet a minimum set of criteria.

Click on the **PEST Check** button on the toolbar. If there are errors, you will receive a notification. (if there are just warnings, you will not receive a notification)

Click the Run PEST button to start the pest.exe. The progress should appear in a DOS window.



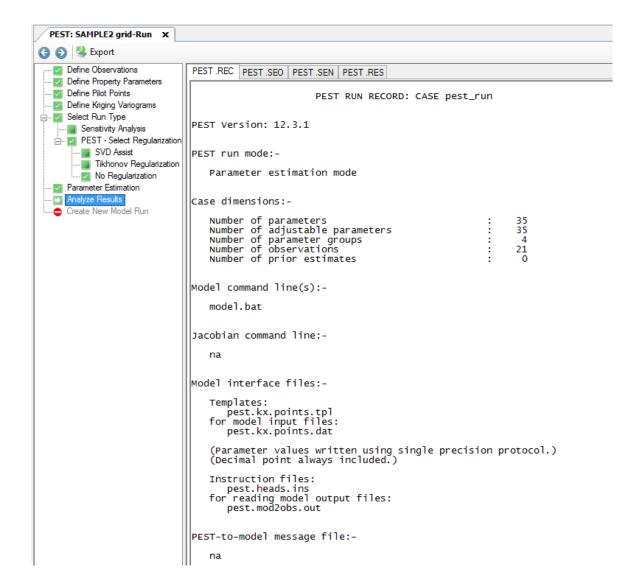
Once PEST finishes, you should see a confirmation message appear under the PEST Run Log tab, indicating if the PEST run was successful or not.

Click Vert Step) to proceed to the <u>Analyze Results</u> step.

14.7 Analyze Results

After the PEST run is successful, you can analyse the results; Visual MODFLOW Flex provides a link to the PEST output files:

- Record file (.REC)
- Sensitivities for Observations (.SEO)
- Sensitivities for Parameters (.SEN)
- Residuals (.RES)



The Analyze Results workflow window includes several tabs which display the output files from the PEST run (i.e. .REC, .SEO, .SEN and .RES files).

The .REC tab displays the **Record File** for the PEST run. The record file includes detailed record of the entire parameter estimation process, listing the number of parameters, parameter groups, observations, parameter definitions/settings, control settings, initial

conditions, etc. The record file also lists the parameter values for each iteration of the model.

The .SEO tab displays the **Observation Sensitivity** file. This file records the sensitivity of each individual observation with respect to all parameters involved in the PEST run. Observed and modeled values are listed for each observation point/time, along with the composite sensitivity of each observation point/time with respect to the estimated parameters.

The .SEN tab displays the **Parameter Sensitivity** file. This file records the sensitivity of each individual parameter with respect to all observations involved in the PEST run. The parameter value and sensitivity are listed for each iteration of the PEST run.

Finally, the .RES tab displays the **Residual file**. This file displays the measured and modeled values for each observation point based on the BEST results achieved by PEST (i.e. the model iteration with the lowest Φ (phi) value. In addition, the residual value for each observation is displayed.

The PEST output files can be exported to Excel spreadsheets for further processing and

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charting. Click on the button to specify an output name/location for the Excel file; the results will be separated into individual worksheets for facilitate analysis.

14.8 Save PEST Parameters as New Inputs

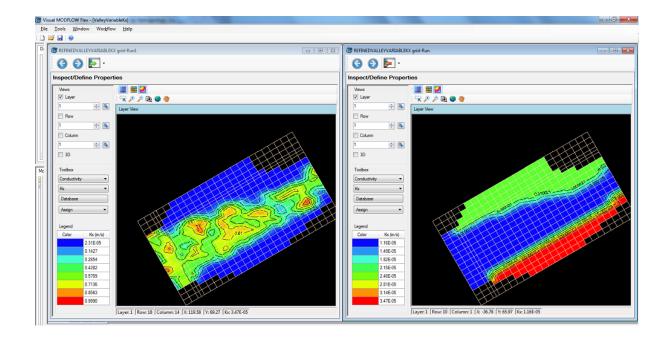
At the end of a PEST run (other than a Sensitivity Analysis), you may want to save the final parameters as inputs for a new model run, provided the adjusted parameters are reasonable.

PEST: SAMPLE2 grid-Run X		
G 🖯		
 Define Observations Define Property Parameters Define Pilot Points Define Kriging Variograms Select Run Type Sensitivity Analysis Sersitivity Analysis SVD Assist Tikhonov Regularization No Regularization Parameter Estimation Analyze Results Create New Model Run 	Create New Model Run Create N	ew Model Run With PEST Results

Click on the "Update Model with PEST Results" button.

Visual MODFLOW Flex will save the adjusted model parameters in a new model run within the same project. This new model run will appear in the Model Explorer below the most recent model run. You must Translate and Run this new model run in order to see the updated MODFLOW results.

In the past, you would need to do a "Save Project As...", if you wanted to keep the original model separate from the PEST updated model. With Visual MODFLOW Flex, you can have all these model scenarios/runs accessible within a single project, allowing you to efficiently compare the original model to the "PEST-adjusted" model run, where you can make comparisons between calculated heads, property zone parameters, etc.



14.9 Making Changes after a PEST Run

After PEST has been run to completion, you may need to make changes to the defined PEST inputs, and/or the numerical model. Please follow the steps below in the case of these changes:

Numerical Model

If you change the model engine, you must go back to the start of the PEST workflow, and click Apply and Next at each step right up to the Run PEST step

If you change the Translation settings (e.g. Solver, Package settings) and or the property package (LPF vs BCF), just go back to the Define Kriging parameters step, click [Apply] button, then you can go directly to Run PEST.

If you need to change the parameter zonation (e.g. add or remove Conductivity zones), this is something that is not yet updated in the PEST workflow. Please make a clone of the model run, change the parameter zonation in this clone, then launch a PEST run from this model clone.

PEST Inputs

If you change the Observations and/or Weights:

- Return to this step in the PEST workflow and make the necessary changes
- Click [Apply] button at the top of the workflow toolbar
- Go to the Run PEST step

If you change the Property Zone parameter min/max values

- Make the changes at this step in the workflow
- Click [Apply] button
- Go to Define Kriging Variograms, and click [Apply] to re-generate these PEST input files.
- Go to the desired regularization step, and Regenerate the PEST Control file.
- Go to the Run PEST step and Run PEST.

If you change the pilot point values, or add new pilot points

- Make the changes at this step in the workflow
- Click [Apply] button
- Go to Define Kriging Variograms, and click [Apply] to re-generate these values
- Go to the Run PEST step.

15 Working with Multiple Model Scenarios

One of the unique features of VMOD Flex is the ability to work with multiple numerical models inside a single project. Unlike other modeling GUI's, VMOD Flex does not restrict you to a single model scenario or single grid for your model. With the workflow based approach, you can generate multiple grid realizations from your conceptual model, each one with one or more model runs. Likewise, you can import multiple MODFLOW models or Visual MODFLOW projects into a single project, and analyze and compare these projects.

Loading a New Workflow

There are a number of ways in which a new numerical model workflow window will be created:

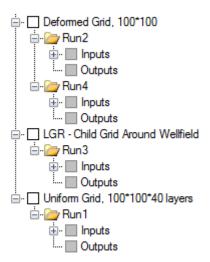
- You have <u>Imported a MODFLOW or Visual MODFLOW project</u>, immediately after creating a new project.
- You have imported an additional MODFLOW or Visual MODFLOW model into an existing project. To use this option, select the Workflow/Numerical Model menu option
- You have "Duplicated" or Cloned an existing numerical model, through the Clone option. To use this option, right click on the "Run" node on the model tree, and select "Clone". When this option is selected, the model run tree in the model explorer will be duplicated, and a new workflow window will appear
- When you are within the Conceptual Model workflow, upon running the <u>Conceptual to</u> <u>Numerical Model</u> conversion.

Each new workflow will load as a separate window inside the VMODFlex main application window.

The windows can be accessed from the window toolbar at the top of the screen, as highlighted in red below.

3D	Viewer - 1	х	Conceptual Model 2	х	UnstructuredGrid1-Run1	×	NumericalGrid1-Run2	x	
96		-	Stop						

The tree structure for multiple model runs is shown below. Each numerical grid (which is derived from a conceptual model) can have one or more model Runs; each model run contains the inputs and output for a single numerical model.



Closing/Minimizing Workflow Windows

You can close a workflow window at anytime by selecting the X button in the top right; however, this is only recommended if you do not need the workflow window until a later time (for example a specific model run).

How To Reload a Closed Workflow

You can reload a workflow window at any time from the Workflow menu, by selecting Workflow/Open, and the following dialog will appear:

	Open Workflows	×
Concep Unstruc Numerio	Workflows to Open: tual Model 2 [Conceptual Workflow] turedGrid1-Run1 [USG Workflow] calGrid1-Run2 [Numerical Workflow] RT-TRANSIENT grid-Run [Numerical Workflow]	w]
	OK Cancel	

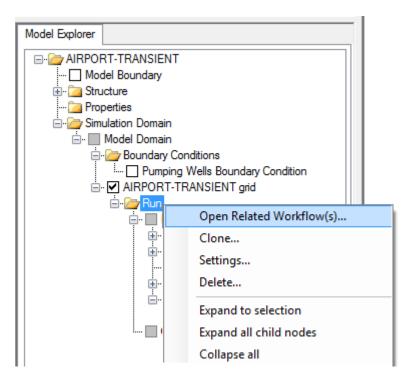
Select the desired workflow(s) and click [OK].

In addition, you can load a specific workflow through the model.

To reload a Conceptual Model workflow, right click on the Conceptual Model node in the model tree, and select Open Related Workflows...

Model Explorer	
B- C AIRPORT-TRANS	ENT
···· 🔲 Model Bound	Settings
Structure	Delete
Zones	Translate to Finite Element Model
📴 Properties	Open Related Workflow(s)
i⇔i i i i i i i i i i i i i i i i i i i	Expand to selection
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	Collapse all

To reload a Numerical Model workflow, right click on the desired **Run** node in the model explorer, and select Open Related Workflow



16 References

Online Guides to USGS Versions of MODFLOW and associated packages:

Engine	Reference Link
MODFLOW-	https://water.usgs.gov/nrp/gwsoftware/modflow2000/Guide/index.htm
2000: MODFLOW-	l https://water.usgs.gov/nrp/gwsoftware/modflow2005/Guide/index.htm
2005:	https://water.usgs.gov/htp/gwsoftware/mounow2005/Guide/index.htm
MODFLOW- NWT:	- https://water.usgs.gov/ogw/modflow-nwt/MODFLOW-NWT-Guide/
MODFLOW-	https://water.usgs.gov/ogw/modflow-lgr/MODFLOW-LGR-
LGR: MODFLOW-	Guide/index.htmlhtml
USG:	https://water.usgs.gov/ogw/mfusg/html
MODFLOW-6:	https://www.usgs.gov/software/modflow-6-usgs-modular-hydrologic- model
MT3D-MS:	https://hydro.geo.ua.edu/mt3d/index.htm
RT3D:	https://www.pnnl.gov/projects/multi-species-reactive-transport- simulation-software-groundwater-systems
SEAWAT:	https://www.usgs.gov/software/seawat-computer-program- simulation-three-dimensional-variable-density-ground-water-flow

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17 Appendix A - Input files and Packages

When you "Translate" in the numerical model, a number of text files will be created; these input files (called packages) are required for the numerical models (engines) to run. These files are saved in the "Run" directory for the current grid/run that you have selected, in the data repository; for example:

\Drumco.data\MODFLOW\NumericalGrid1\Run\MODFLOW-NWT\..

If you choose a different engine (at the "Select Engines" step), then a new folder will be created under that run.

In Visual MODFLOW Flex, most of the packages containing arrays will have a main "index" file which lists global settings/parameters and provides file references to the other files that are also inputs for that package. An example is the MODFLOW .DIS package; some general parameters (such as units) and temporal discretization (number of stress periods and time steps) are described in this projectname.DIS file; however, cell elevations for each layer are described in their own separate file, for example Projectname.DIS.Bot1 (contains bottom elevations for each cell, for layer 1)

A brief description of these files is listed below, where projectname is the name assigned to the model.

MODFLOW (2000, 2005, NWT)

A brief description of these files is listed below, where projectname is the name assigned to the model.

Input files:

- projectname.modflow.IN List of translated files for MODFLOW
- projectname.BAS: Basic Package data file
- projectname.BCF: Block-Centered Flow Package data file.
- projectname.CHD: Time-variant specified head data file
- projectname.DIS: Model discretization data file
- projectname.DRN: Drain Package data file
- projectname.EVT: Evapotranspiration Package data file.
- projectname.FHB: Flow and Head Boundary Package data file.
- projectname.GHB: General-Head Boundary Package data file
- projectname.HFB: Horizontal Flow Boundary Package data file.
- projectname.LPF: Layer Property Flow data file
- projectname.MNW: Multi-Node Well (1/2) Package data file
- projectname.MNWI: Multi-Node Well Input/Output data file
- projectname.OC: Output control options data file
- projectname.PCG: PCG2 Solver Package data file
- projectname.RCH: Recharge Package data file
- projectname.RIV: River Package data file

- projectname.SFR: Streamflow-Routing Package data file
- projectname.SIP: SIP Solver Package data file
- projectname.SOR: SOR Solver Package data file
- projectname.UZF: Unsaturated Zone Flow Package date file
- projectname.WEL Well Package data file
- projectname.WHS: WHS Solver data file

Input Packages specific to MODFLOW-NWT:

- projectname.UPW: Upstream Weighting (property package, only when MODFLOW-NWT is selected)
- projectname.NWT: NWT Solver settings (this solver must be used when MODFLOW-NWT is selected)

Input Packages specific to MODFLOW-USG:

- projectname.CLN: connected linear network package file
- projectname.GNC: Ghost-node correction package, which includes additional node coordinate information facilitate corrections for cell geometries that do not inherently satisfy the requirements of the flow formulation in MODFLOW-USG
- projectname.GSF: Grid Specification file, which includes grid cell vertex coordinates and connectivity
- projectname.SMS: Sparse Matrix Solver package file

Output files:

- projectname.BGT* MODFLOW file containing water budget data used by MODPATH
- projectname.CBB* MODFLOW-SURFACT file containing water budget data used by MODPATH (Binary format)
- projectname.CBC* MODFLOW-USG file containing water budget data used by MOD-PATH3DU (Binary format)
- projectname.DDN MODFLOW file containing drawdown X, Y, Z heads for each node (Binary format)
- projectname.FLO* MODFLOW file containing cell-by-cell flow terms (Binary format)
- projectname.HDS* MODFLOW file containing head results (Binary format)
- projectname.LST* MODFLOW listing file containing information and messages from MODFLOW (ASCII format)

MODFLOW-6

A brief description of these files is listed below, where projectname is the name assigned to the model.

Input files:

Simulation Files

- mfsim.nam: simulation composition including options and links to models, time discretization, model exchanges, and solution group information
- projectname.tdis: simulation time discretization package data

Groundwater Flow (GWF) Model files:

- .\GWF\projectname.NAM list of translated files for the flow model and related options
- .\GWF\projectname.IMS: iterative matrix solution package data containing solver settings
- .\GWF\projectname.DIS(V): grid discretization (by vertices) package data containing grid information
- .\GWF\projectname.IC: initial condition package data containing starting heads
- .\GWF\projectname.OC: output control package data containing information on which data to include in the outputs and for which time steps
- .GWF\projectname.NPF: node property flow package data containing conductivities
- .\GWF\projectname.STO: storage package data containing transient storage parameters
- .\GWF\projectname.{boundary condition name}.EVT: evapotranspiration package data file
- .\GWF\projectname.{boundary condition name}.RCH: recharge package data file
- .\GWF\projectname.{boundary condition name}.CHD: time-variant specified head file (one per Constant Head boundary condition in the model tree)
- .\GWF\projectname.{boundary condition name}.DRN: drain package data file (one per Drain boundary condition in the model tree)
- .\GWF\projectname.{boundary condition name}.GHB: general head package data file (one per General Head boundary condition in the model tree)
- .\GWF\projectname.{boundary condition name}.RIV: river package data file (one per River boundary condition in the model tree)
- .\GWF\projectname.{boundary condition name}.WEL: well package data file (one per Well boundary condition in the model tree)

Groundwater Transport (GWT) Model files: (one set of files per species {S001}, if applicable)

- .\GWT\{S001}\projectname.NAM list of translated files for the transport model and related options
- .\GWT\{S001}\projectname.IMST: iterative matrix solution package data containing solver settings for the transport solution
- .\GWT\{S001}\projectname.DIS(V): grid discretization (by vertices) package data containing grid information
- .\GWT\{S001}\projectname.IC: initial condition package data containing starting concentrations
- .\GWT\{S001}\projectname.OC: output control package data containing information on which data to include in the outputs and for which time steps
- .GWT\{S001}\projectname.ADV: advection package data
- .\GWT\{S001}\projectname.DSP: dispersion package data containing mechanical dispersion and diffusion values
- .\GWT\{S001}\projectname.MST: mobile storage and transfer package data containing porosities, retardation, and reaction parameter values for the mobile domain
- .\GWT\{S001}\projectname.IST: immobile storage and transfer package data containing porosities, retardation, and reaction parameter values for the immobile domain (up to three immobile domains may be specified)
- .\GWT\{S001}\projectname.SSM: source-sink mixing package data containing a list of boundary condition from the flow model with (auxiliary) concentrations

- .\GWT\{S001}\projectname.CNC: constant concentration package data file (one per constant concentration boundary condition in the model tree)
- .\GWT\{S001}\projectname.SRC: mass source loading package data file (one per constant Mass Flux boundary condition in the model tree)

Output files:

Simulation Files:

• mfsim.lst: simulation progress and diagnostic listing file

Groundwater Flow (GWF) Model:

- .\GWF\projectname.lst: groundwater flow model progress and diagnostic file
- .\GWF\projectname.hds: file containing output heads (Binary format)
- .GWF\projectname.bgt: file containing output cell-by-cell flows/budgets and used to calculate velocity vectors (Binary format)
- .\GWF\projectname.ddn file containing output drawdown values (Binary file generated by Visual MODFLOW Flex)

Groundwater Transport (GWT) Model: (one set of files per species {S001}, if applicable)

- .\GWT\{S001}\projectname.lst: groundwater flow model progress and diagnostic file
- .\GWT\{S001}\projectname.hds: file containing output heads (Binary format)
- .\GWT\{S001}\projectname.bgt: file containing output cell-by-cell flows/budgets and used to calculate velocity vectors (Binary format)
- .\GWT\{S001}\projectname.ddn file containing output drawdown values (Binary file generated by Visual MODFLOW Flex)

MODPATH

Input files:

- BACKWARD.IN Backward tracking particle locations data file
- BACKWARD.PTH Backward tracking run options data file
- FORWARD.IN Forward tracking particle locations data file
- FORWARD.PTH Forward tracking run options data file
- projectname.MPT Main MODPATH input data file
- MODPATH.IN List of MODPATH input files

Output files:

- projectname.CBF Composite Budget file used by MODPATH
- projectname.MPB MODPATH file containing backward tracking particle information (ASCII format)
- projectname.MPF MODPATH file containing forward particle information (ASCII format)
- SUMMARY.PTH* MODPATH file containing listing information and messages from MODPATH (ASCII format)

MOD-PATH3DU

Input files:

- Conceptual Model.JSON Primary input file in JavaScript Object Notation (JSON) format
- Conceptual Model.MP3DU.GSF grid specification file compatible with MOD-PATH3DU
- Conceptual Model.MP3DU.IN model input file
- Conceptual Model.P3D model property file
- One set of files per input particle group:
 - Conceptual Model_{pathiline group}.shp shapefile with particle group starting location coordinates
 - Conceptual Model_{pathiline group}.dbf shapefile database with particle group attributes
 - Conceptual Model_{pathiline group}.shx shapefile spatial index

Output files:

- MP3DU.log output listing file in JSON format
- One set of files per corresponding output pathline group:
 - Conceptual Model_{globally_unique_id}.PATHLINE.BIN binary output file with particle group pathlines
 - Conceptual Model_{globally_unique_id}.PATHLINE.shp shapefile with particle group pathlines
 - Conceptual Model_{globally_unique_id}.PATHLINE.dbf shapefile database with pathline attributes
 - o Conceptual Model_{globally_unique_id}.PATHLINE.shx shapefile spatial index

MT3DMS / RT3D / SEAWAT

Input files:

- projectname.AD3 Advection data file
- projectname.BT3 Basic Transport data file
- projectname.DP3 Dispersion data file
- projectname.GCG Transport Solver data file
- projectname.RC3 Chemical Reaction data file
- projectname.SS3 Source / Sink Mixing data file

Packages specific to MT3DMS:

• MT3D.IN List of MT3D input files

Packages specific to RT3D:

• RT3D.IN List of RT3D input files

Packages specific to SEAWAT:

- SEAWAT.IN List of SEAWAT input files
- projectname.VDF Variable Density Flow data file
- projectname.VSC Viscosity data file

Output files:

- projectname.OT* MT3D output file containing listing information and messages from MT3D e.g. cumulative mass budget data (ASCII format)
- projectname.CNF* MT3D file containing model grid configuration file (ASCII format)
- projectname.MAS* MT3D file containing mass balance file (ASCII format)

Please Note: The mass balance files are displayed by MS-Windows as projectname.001, projectname.002, etc.

- projectname.OBS* MT3D file containing concentration at observation points (ASCII format). The data is presented with units of mass/length^3
- projectname.UCN* MT3D file containing unformatted concentration information -(Binary format)

ZONEBUDGET

Input files:

- projectname.ZBI Zone Budget data file
- ZONEBUD.IN List of Zone Budget input files

Output files:

• projectname.ZOT Zone Budget file containing water balance data (ASCII format).

18 Appendix B - VM Flex GUI and Input Files

MODFLOW (2000, 2005, NWT)

A brief description of these files is listed below

BAS: Basic Package

Array data originates from various spots in the Input:

- View/Edit Grid (Active/Inactive cells)
- Properties / Initial Heads
- Define Boundary Condition (Constant Heads only, steady state only)

Some settings are defined at Translate step, check the Initial Heads option.

Reference files in this package may include the following external array files (one each per layer, with the digit suffix representing the layer index):

OPEN/CLOSE Name.BAS.ibound1 Active flag for each cell: active, constant head, or inactive

OPEN/CLOSE Name.BAS.head1

Initial head value for each cell; the values will depend on what option you chose for Initial Heads at the Translate step.

DIS: Discretization Package

Contains the spatial and temporal discretization; also contains the units. Array data originates from Input, View/Grid (# rows, cols, layers, layer top, layer bottom). Some settings are defined at Translate step, Time Steps. Units are defined in Proj settings. # Stress periods is based on the boundary conditions in the input.

The first set of arrays contains the cell width. The second set of arrays contains the cell height.

Please Note: These only need to be defined once, since all layers in a finite difference model must have same cell width and height

After that are links to the cell elevation for each layer.

OPEN/CLOSE Name.DIS.Top' 1 (FREE) -1 #Top Elevation The cell top elevation value for cells in layer 1

OPEN/CLOSE Name.DIS.Bot1' 1 (FREE) -1 #Bottom Elevation of layer 1 The cell bottom elevation value for layer 1

Property Packages

BCF: Block Center Flow package

Used for MODFLOW-2000 and 2005

Array data originates from Input/Properties. Conductivity and Storage.

Some additional settings are defined at Translate step, mainly using the Layer types, Rewetting, and Anisotropy options.

Details on the Referenced files from within this package are explained below:

Starting at line 5:

OPEN/CLOSE Name.BCF.ss1' 1 (FREE) 0 #Ss (specific storage) for layer 1 (this file will contain cell-by-cell values for specific storage, for layer 1)

OPEN/CLOSE Name.BCF.hk1' 1 (FREE) -1 #HK for layer 1 (this file will contain cell-by-cell values hydraulic conductivity values for layer 1)

OPEN/CLOSE Name.BCF.vcont1' 1 (FREE) 0 #VCONT for layer 1 (this file will contain cell-by-cell values VCONT values for layer 1)

If you have enabled additional options such as Anisotropy "As Specified" or Cell Re-wetting, you may see references to additional parameters.

LPF: Layer Property Flow Package

Same as BCF; the main difference is that Kz is explicitly defined (there are no values for VCONT or Transmissivity)

OPEN/CLOSE 'Conceptual Model 1.LPF.hk1' 1 (FREE) -1 #HK for layer 1 (this file will contain cell-by-cell values for Horizontal Conductivity (Kx) for layer 1)

OPEN/CLOSE 'Conceptual Model 1.LPF.vka1' 1 (FREE) -1 #VKA for layer 1 (this file will contain cell-by-cell values for Vertical Conductivity (Kz) for layer 1)

OPEN/CLOSE 'Conceptual Model 1.LPF.wetdry1' 1 (FREE) -1 #Wetdry for layer 1 (this file will contain wet dry flags for layer 1)

UPW: Upstream Weighting Package

Same format as LPF package. Used for MODFLOW-NWT only.

Boundary Conditions

These are specified at the "Define Boundary Conditions" step in the numerical modeling workflow.

The following boundary conditions use format "Layer, Row, Column, parameter," in their package (and do not use arrays)

Constant Head

- River
- General Head
- Drain
- Wall (HFB)
- Specified Flux
- Wells

The format of these packages is described in the USGS MODFLOW documentation. The remaining boundary conditions in VMOD Flex require defining values in one or more arrays. These are described below.

Recharge (RCH)

Array data originates from Input, Define Boundary Conditions/Recharge and EVT.

Some settings are defined at Translate step, Recharge.

Name.RCH.recharge0' 1 (FREE) -1 #Recharge Contains cell-by-cell recharge rate for stress period 1.

Name.RCH.recharge1' 1 (FREE) -1 #Recharge Contains cell-by-cell recharge rate for stress period 2.

***This is repeated for subsequent stress periods for a transient simulation

Evapotranspiration (EVT)

Array data originates from Input, Define Boundary Conditions/Evapotranspiration.

Some settings are defined at Translate step, Recharge and EVT.

In the input (click on database), you define the following parameters:

- Evapotranspiration Rate
- Extinction Depth

Name.EVT.elevation' 1 (FREE) -1 #Elevation Contains the ground elevation values for layer 1

Name.EVT.evapotranspiration0' 1 (FREE) -1 #Evapotranspiration Contains the evapotranspiration rate for each cell, for stress period 1. ***This is repeated for subsequent stress periods for a transient simulation

Name.EVT.depth0' 1 (FREE) -1 #Extinction Depth Contains the exctinction depth values for each cell, for stress period 1 ***This is repeated for subsequent stress periods for a transient simulation

Lake (LAK)

Array data originates from Input, Define Boundary Conditions/Lakes

Some settings are defined at Translate step, "Lakes"

Name.LAK.lkarr1' 1 (FREE) -1

Active/inactive cells; for any cell that is defined with a lake, it must be marked as inactive.

Name.LAK.bdlknc1' 1 (FREE) -1 #Lake bed leakance for layer 1 Lake bed leakance for each cell, for layer 1. This is calculated from the parameters defined for the lake at the Boundary conditions step.

ZONEBUDGET

.ZBI contains the array of cells, and what zone ID is assigned to each cell. All layers are contained within a single file.

MODPATH

.MPT file is the main input file; it contains some general information at the top.

Details on the Referenced files from within this package are explained below:

OPEN/CLOSE 'Conceptual Model 1.MPT.ibound1' 1 (FREE) -1 Active/inactive flag for cells, for layer 1. (the values are the same as those in the .BAS package)

OPEN/CLOSE 'Conceptual Model 1.MPT.ep1' 1 (FREE) -1 #Ep (Effective Porosity) for layer 1

Effective porosity values for each cell, for layer 1. These values originate from the Define Properties step, "Storage" parameters.

MT3DMS / RT3D / SEAWAT

AD3 Advection

Advection schme and settings; defined at the Translation step, MT3DMS Translation settings

BT3 (Basic Transport)

Contents of this file:

- Cell column data (cell width): this is based on the cell dimensions. There is just one array for all layers in the model
- Cell row delta (cell height): same as above
- Htop/water table elevation: Top elevation of the cell, or the water table elevation, whichever one is higher. There is just one array.

You can find this by looking at the cell dimensions at the Input/Grid step

• Layer Thickness: one array per layer. This is based on the cell height. You can see this at the view/edit grid step.

- Porosity: one array per layer. Input for this is defined at Define Properties/Storage. (**note:** Total [default] or effective porosity can be selected here)
- icbund: active/inactive cells for layer 1. (1=active, 0=inactive)
- Starting Conc. (SCONC) Layer 1: at Define Properties/Initial Concentration step.

Also contains the "saved" output times for the MT3DMS run; these are defined at the Translate step, under MT3DMS node.

DP3 (Dispersion)

Contains the Dispersion parameters; these are defined at the Define / Properties step, Long. Dispersion.

RC3 (Chemical Reactions)

Contains the chemical reaction parameters; these are defined in Flex as "Species Parameters" and "Model Parameters". Default values and some global parameters are defined at the Define Modeling Objectives step; cell-by-cell values for model parameters and species parameters are defined/assigned/edited at the Define Properties step.

SS3 (Sinks / Sources)

Contains the Sink/sources (transport boundary conditions). These are defined at the "Define Boundary Conditions" step; these can be Constant Concentration, concentrations assigned to Pumping Well rates, or can be species concentrations for existing boundary conditions such as River, Recharge, EVT.

GCG Solver

Solver parameters and time steps; defined at the Translation step, MT3DMS/RT3D/SEAWAT Translation settings

SEAWAT Only

VDF (Variable Density Flow)

Contains the variable density settings and parameters; some of these parameters are defined at the Define Modeling Objectives step; settings and a few relevant parameters are set using the advanced Transport Engine settings at the Translation step.

VSC (Viscosity)

Contains the viscosity package settings and parameters; some of these parameters are defined at the Define Modeling Objectives step; cell-by-cell values are defined at the Define Properties step; settings and a few relevant parameters are set using the advanced Transport Engine settings at the Translation step.

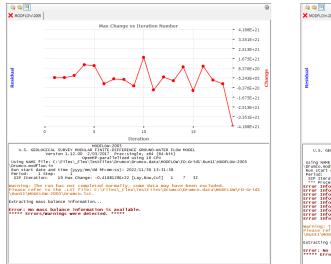
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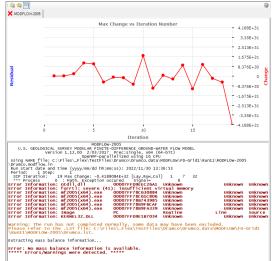
Model Non-Convergence and Stability - Flow Engine Runs

If you are experiencing difficulty in getting your model to run successfully, you may be running into issues with model stability (e.g. output heads or concentrations exceed an absolute value of 1E+30) and/or model convergence (e.g. the simulation exceeds the specified number of solver iterations). These issues can often be solved by examining your model and making a number of common adjustments to your model inputs and run settings. We recommend that you read through the following suggestions, and apply them to your model, where applicable and appropriate. Please remember that in many cases, a combination of changes to your model may be required to reach stability and convergence.

Stability

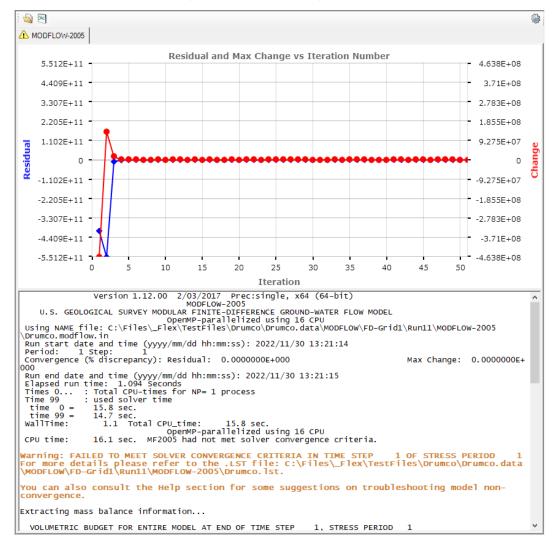
Model stability issues occur when the solution converges towards plus/minus infinity (or absolute values greater than the min/max number allowed by most engines is approximately 10³⁸). This will typically be indicated during a run by a red "X" in the Engine Tab and either a red "no mass balance information" error (as shown below on the left) or a crashed engine (as shown below on the right) when one or more values in the model exceeds the maximum allowed value.





Non-Convergence:

Model non-convergence occurs when the numerical solver does not find a solution to the specified level of precision of the closure/convergence criteria within the allotted number of solver iterations. This will typically be indicated during a run by warning sign in the



Engine tab at the Run step and by an orange warning message in the console output (note, this will occur near the top of the console output):

Here are some things to check when your model run does not complete successfully:

Potential Issue #1: Solvers and Settings

The default solver settings for <u>flow</u> and <u>transport</u> models in Flex are typically sufficient for most simple models. However, more complex models may require some adjustments to the solver settings to reach convergence. If the model almost converges, (i.e. the output global mass balance error reported in the run console is relatively low), you can try increasing the number of inner/outer iterations to provide the numerical algorithms a little more "time" to reach convergence and/or adjust the convergence criteria (called HCLOSE and/or RCLOSE in most solvers). You may also try experimenting with different solvers and their more advanced settings.

Potential Issue #2: Initial Heads for Steady-State runs are not close enough to a stable solution

In theory, the specified initial heads for steady should have no impact on the resulting heads for a steady-state simulation; however, in practice, the values of the initial heads can affect how hard the numerical solver may have to work to reach a solution and even lead to non-convergence or stability issues, in some cases, particularly if the initial guess is too far from equilibrium. For steady state simulations, if possible, you should attempt to set initial heads relatively close to the expected steady state values. Luckily there are a few tools that help you with with this:

- 1. You can try settings the <u>Initial Heads</u> to use ground surface elevation or use a previous MODFLOW run for the same model under different condition (if available).
- If you have multiple observed/expected heads (including from surface waters), you can interpolate these to <u>create</u> potentiometric surfaces for each aquifer in your model
- 3. You can use the <u>Expression Builder</u> to develop a surface that approximates the expected location of the water table (e.g. it occurs 2m below the ground surface or at elevations corresponding to 75% saturation of the upper-most model layer)

Potential Issue #3: Water Table Issues (Dry cells in your model domain and/or pumping wells that are running dry)

Most of the MODFLOW flow engines included with Visual MODFLOW Flex are designed to simulate saturated flow conditions only. If you have large areas of your model that are above the water table, or areas where the water table is dropping below or straddling model layers, the resulting dry cells can result in convergence problems.

Additionally, if areas are cycling between saturated and unsaturated (wet and dry) conditions due to water table fluctuation, Recharge settings, or Rewetting settings, this can also cause convergence problems due to oscillation.

- Check to see that you have entered an appropriate Recharge value for your model, and that it is assigned to the "highest active layer" (at the Translation step, select the Recharge and EVT settings node, under the MODFLOW-flow engine branch and try adjusting the settings for the NRCHOP and NEVTOP options.
- If you think that Rewetting is causing oscillation in your model, try reducing the Wetting interval to every 3-5 iterations, or switch to MODFLOW-NWT, which has a more robust formulation (.UPW) and solver (.NWT) approach that avoid WET/DRY cells.
- 3. Consider re-assigning layer elevations, or combining the top layers in your model, to increasing the layer thickness, and reduce the probability of dry cells. Visual MODFLOW is largely a saturated flow-modeling program. If you have layers above your water table, they will become Dry during the model run, which can cause non-convergence. You may receive an error message referring you to the .LST file.
- 4. If drawdown around pumping wells is causing wells to run dry, convergence problems can surface. You may need to revise your model inputs (e.g. conductivity

values, layer thickness(es), pumping rates/screen elevations, grid discretization, etc.) to keep the cell(s) in which the well is assigned from going dry.

If you are not able to resolve dry cell issues in your model, you may want to consider using the MODFLOW-NWT Flow Engine. This engine is a special version of MODFLOW-2005 and was specifically developed by the USGS to improve solver performance for problems involving drying and rewetting nonlinearities of the unconfined groundwater-flow equation.

Another option to consider, particularly if you need improved evaluations of the location of the water table and/or unsaturated flow, is MODFLOW-SURFACT. This add-on package for Visual MODFLOW Flex is designed to simulate Unsaturated and Saturated conditions without difficulty, and is also capable of handling wells screened over multiple layers where one or more layers are being pumped dry, perched water tables, steep water table gradients, and other complex project scenarios. You can contact the Waterloo Hydrogeologic Sales department at <u>sales@waterloohydrogeologic.com</u> or +1 519-746-1798, for more information on the MODFLOW-SURFACT Flow Engine.

If you have checked the previous common problems, and implemented the solutions, yet your model will still not converge, you may want to consider adjusting the parameters of your solver, or trying a different solver (see Potential Issue #1 above).

Potential Issue #4: Imbalanced Boundary Conditions

Check the mass balance in the MODFLOW listing file to see if boundary conditions are unbalanced. A common source of convergence issues, particularly in steady-state models, is that source boundary conditions are out of balance with sink boundary conditions, and/or the conductance of the model. That is the model may be adding more water than can move through the model or can be removed by the specified sinks OR the model may be removing more water than can move through the model or than is being added by the specified sources.

- 1. Check the run console (or the contents of the model .LST file) for the volumetric budget for the entire model and verify whether there are any boundary conditions with unexpectedly high/low values and adjust model inputs as necessary. If the model is steady state is not stable so that no results are produced; you may try to set the model to run as transient for a very short duration to force an output mass balance to see which boundary conditions are adding/removing unexpected amounts of water to the model particularly relative to other boundary conditions
- 2. Similarly, boundary conditions may be out of balance with nearby inter-cell conductances, which are composed of hydraulic conductivity, and cell dimensions (please refer to the documentation/development of the specific groundwater flow package (e.g. BCF, LPF, UPW, etc.) in the original user manual for the applicable engine for how conductances are calculated). Certain boundary conditions, particularly Type-2 boundary conditions which have a specified flux (e.g. recharge (RCH), well (WEL), and specified flux (FHB)), may add or remove more water than the inter-cell conductances of nearby cells can accommodate with a stable numerical solution. Check the input values of these types of boundary conditions relative to nearby conductances. In particular, check recharge rate values, noting that recharge is applied at a constant rate, regardless of the receiving conductivity.

Stability/convergence issues may occur when the specified recharge rate exceeds the vertical hydraulic conductivity in the cell(s) where it is applied. It may be useful to start with little to no recharge at first and increase the rate(s) incrementally.

3. Similarly if heads around certain boundary conditions are excessively high/low, this may be caused by inappropriate values/assignment locations. You may need to revise your model inputs. Note that, most boundary conditions (including drains (DRN), rivers (RIV), wells (WEL), general heads (GHB), etc.) will be deactivated by MODFLOW in cells that run dry. This can cause oscillatory behavior (i.e. repetitive decline and recovery of the water table across model layers), particularly when cell rewetting is active (see potential issue #3 above)

Potential Issue #5: Sharp gradients in the grid

Stability and non-convergence issues may occur in models with abrupt changes in the grid properties leading to sharp gradients in inter-cell conductance, which can be problematic for the numerical solution methods incorporated in the MODFLOW engines:

- 1. Models with abrupt changes of the hydraulic conductivity between adjacent cells (e.g. differences of many orders of magnitude), may lead to stability issues. Try to reduce the numerical difference in hydraulic conductivities between neighboring cells, or insert additional conductivity zones to smooth the transition between large gradients in hydraulic conductivity.
- 2. Models with large differences in the cell dimensions between adjacent cells, may lead to stability issues. As a rule of thumb, grid spacing should not increase by more than 50 percent between adjacent cells. As well, an aspect ratio must generally be respected: a grid cell should not be more than 10 times larger in one direction than in another. You may want to <u>edit</u> the refinement(s) in your grid in problematic sections.
- 3. Models with lateral discontinuities between cells in the same layer. may lead to numerical issues: Large changes in elevation (especially when your model has thin layers) can cause adjacent cells to become laterally "detached", resulting in a lack of lateral continuity. This may introduce significant inaccuracies when simulating flow between cells in the same layer. Avoid this by reducing large changes in elevation over short distances, and/or refining your grid, and/or changing layer thickness. As a rule of thumb, adjacent cells in the same layer should overlap 50% of their "depth" (along the Z axis). You can use the View Row and View Column tools in Visual MODFLOW Flex to study areas in cross-section.

While the incorporating some above suggestions may help to fix some common causes of model non-convergence and stability, they are not a panacea and do not cover every situation. If these suggestions do not help you successfully run your model, additional thought may need to be put into your modeling conceptualization and numerical implementation, that is the non-convergence may be indicative of one or more defects in the conceptualization of the groundwater system.

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