# Process Model Formulation

## Process Models Used in Biowin

BioWin uses a general Activated Sludge/Anaerobic Digestion (ASDM) model which is referred to as the BioWin General Model. The BioWin General Model has fifty state variables and sixty process expressions. These expressions are used to describe the biological processes occurring in activated sludge and anaerobic digestion systems, several chemical precipitation reactions, and the gas-liquid mass transfer behavior for six gases. The model formulation requires pH determination which is described in the pH chapter. This complete model approach frees the user from having to map one model's output to another model's input which significantly reduces the complexity of building full plant models, particularly those incorporating many different process units.

This chapter provides an overview of the model and the parameters included in the model.. In some cases you will be referred to other documents that describe sections of the model in greater detail. In this section the model parameters (kinetic, stoichiometric, settling and chemical constants) are listed in full with a brief description of the model process. Parameters that are of special importance (those having a direct impact on a measurable wastewater, effluent or plant characteristics) are highlighted in the tables.

The default BioWin General Model can be augmented with additional processes or entirely replaced by other models which have been defined in the Model Builder. BioWin includes a library of Model Builder models. Details on the Model Builder are in the **Model Builder** section of the "*Common Dialog*" chapter.

For a list of the models included with BioWin, please see the **Model Library for the Model Builder** section later in this chapter.

## Activated Sludge Model

The activated sludge model in BioWin contains the following functional categories.

**Growth and Decay of Ordinary Heterotrophic Oganisms**

**Growth and Decay of Methylotrophs**

**Hydrolysis, Adsorption, Ammonification and Assimilative denitrification**

**Growth and Decay of Ammonia Oxidizing Biomass**

**Growth and Decay of Nitrite Oxidizing Biomass**

**Growth and Decay of ANaerobic AMMonia OXidizers (ANAMMOX)**

### Growth and Decay of Phosphorus Accumulating Organisms

**Note:** In an activated sludge system, under anaerobic conditions, the anaerobic processes described in the **Anaerobic digestion section** may also have a significant impact.

These modules are described in detail below.

## Growth and Decay of Ordinary Heterotrophic Organisms

**Number of Processes:** 11

**Engineering Objective:** BOD removal, denitrification

**Implementation:** permanent, always active in the BioWin model

**Module Description:**

This group of processes describes the growth of ordinary heterotrophic organisms under aerobic and anoxic conditions and the decay of these organisms under all conditions. The activated sludge model allows for direct ordinary heterotrophic aerobic growth on acetate, propionate, readily biodegradeable complex substrate and methanol. The organisms will tend to use the substrates in the order specified. Under anoxic conditions, the ordinary heterotrophs can use only three of the substrates, namely; acetate, propionate and readily biodegradable complex substrate. In the BioWin model, anoxic use of methanol is restricted to a specialized group of organisms (see anoxic methylotrophs).

The base rate expression for each of the 10 growth processes is the product of the maximum specific growth rate, the heterotrophic biomass concentration and a Monod expression for one of the substrates. This base rate is modified to account for environmental conditions (dissolved oxygen, nitrate and nitrite), nutrient limitations (ammonia, phosphate, other cations and anions), pH inhibition and substrate preference weighting. BioWin uses ammonia as a nitrogen source for cell synthesis with all of the substrates under aerobic, anoxic and anaerobic conditions. At low ammonia concentrations BioWin allows for assimilative ammonia production from either nitrate or nitrite in order to satisfy synthesis demands.

Under anoxic conditions the base rate is also multiplied by the anoxic growth factor and preferentially uses nitrite as the electron acceptor. The decay process has a rate that varies according to the electron acceptor environment.

Model parameters affecting the performance of this module are listed below:

### *Kinetic Parameters*

Menu Location: **Project|Parameters|Kinetic|OHOs**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Max. spec. growth rate | 3.2 | $d^{-1}$ | Determines the maximum specific growth rate of heterotrophs. Substrate and nutrient limitations will decrease the growth rate. This parameter is sensitive only in very |

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| | | | high loaded plants (short SRT), and determines maximum BOD removal capacity. |
| Substrate half sat. | 5.0 | mgCOD/L | This parameter impacts the residual soluble substrate concentration in the effluent. The value is usually low in normal municipal plants. |
| Anoxic growth factor | 0.5 | - | This parameter decreases the maximum specific growth rate under anoxic conditions. Substrate and nutrient limitations may further reduce the growth rate. |
| Aerobic decay | 0.62 | $d^{-1}$ | Decay rate constant under aerobic conditions. This parameter impacts the endogenous respiration rate and VSS destruction during aerobic stabilization. |
| Anoxic/anaerobic decay | 0.3 | $d^{-1}$ | Decay rate constant in the absence of oxygen. |

## *Stoichiometric Parameters*

Menu Location: **Project|Parameters|Stoichiometric| OHOs**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Yield (Aerobic) | 0.666 | mgCOD/mgCOD | Amount of biomass COD produced using one unit of readily biodegradable complex substrate COD. The remaining COD is oxidized. This parameter is very stable in municipal plants and seldom needs adjustment. In case there is a mismatch between measured and simulated sludge production and OUR, try adjusting the influent fup (unbiodegradable particulate COD fraction) parameter or check wastage and SRT. |
| N in Biomass | 0.07 | mgN/mgCOD | N content of heterotrophs. This parameter impacts the nitrogen available for nitrification and therefore oxygen demand. |
| N in Inert | 0.07 | mgN/mgCOD | N content of endogenous residue from heterotrophic decay. |
| P in Biomass | 0.022 | mgP/mgCOD | P content of heterotrophs. This parameter influence the P removal in non bio-P systems, and the P content of the sludge. |
| P in Inert | 0.022 | mgP/mgCOD | P content of endogenous residue from heterotrophic decay. |

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| Endogenous Residue | 0.08 | - | Fraction of biomass that becomes inert upon decay. |
| COD:VSS Ratio | 1.42 | mgCOD/mgVSS | Conversion factor between biomass as measured in COD and its VSS content. This value is relatively stable for biomass. |
| Yield (anoxic) | 0.54 | mgCOD/mgCOD | Biomass yield on readily biodegradable complex substrate COD under anoxic conditions. |
| Yield propionic (aerobic) | 0.5 | mgCOD/mgCOD | Biomass yield on propionic acid COD under aerobic conditions. |
| Yield propionic (anoxic) | 0.41 | mgCOD/mgCOD | Biomass yield on propionic acid COD under anoxic conditions. |
| Yield acetic (aerobic) | 0.4 | mgCOD/mgCOD | Biomass yield on acetic acid COD under aerobic conditions. |
| Yield acetic (anoxic) | 0.32 | mgCOD/mgCOD | Biomass yield on acetic acid COD under anoxic conditions. |
| Yield methanol (Aerobic) | 0.5 | mgCOD/mgCOD | Biomass yield on methanol COD under anoxic conditions. |

## *pH Inhibition*

Menu Location: **Project|Parameters|Kinetic|pH**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Heterotrophs low pH limit | 4.0 | pH units | At a pH equal to this value the growth rate of ordinary heterotrophic biomass will be reduced by 50%. Heterotrophs exhibit tolerance for pH changes – hence the wide pH range. |
| Heterotrophs high pH limit | 10.0 | pH units | At a pH equal to this value the growth rate of ordinary heterotrophic biomass will be reduced by 50%. |

## *Switching Functions*

Menu Location: **Project|Parameters|Kinetic|Switches**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Heterotrophic DO half sat. | 0.05 | $mgO_2/L$ | This constant is used to switch off aerobic OHO activity under low DO conditions (that is in anaerobic and anoxic reactors). |
| Aerobic denit. DO half sat. | 0.05 | $mgO_2/L$ | This constant is used to turn anoxic OHO growth processes on under low dissolved oxygen conditions. [Simultaneous or aerobic denitrification switch.] |
| Anoxic NO3 | 0.1 | mgN/L | This constant is used to switch off anoxic growth processes using nitrate under low |

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| half sat. | | | nitrate conditions. |
| Anoxic NO2 half sat. | 0.1 | mgN/L | This constant is used to switch off anoxic growth processes using nitrite under low nitrite conditions. |
| NH3 nutrient half sat. | 0.001 | mgN/L | This constant is used to slow all biomass growth processes at low ammonia-N concentrations (N nutrient limiting conditions – see assimilative denitrification). |
| P nutrient half sat. | 0.001 | mgP/L | This constant is used to slow the growth of biomass when there is no phosphorus available as nutrient. |
| Synthesis anion/cation half sat. | 0.01 | meq/L | Half saturation concentration for anions and cations. |

## Growth and Decay of Methylotrophs

**Number of Processes:** 3

**Engineering Objective:** denitrification using methanol

**Implementation:** permanent, always active in the BioWin model

**Module Description:**

These processes describe the growth and decay of specialized heterotrophs using methanol under anoxic conditions. In the BioWin model anoxic methylotrophs can only growth under anoxic conditions using methanol as substrate and either nitrate or nitrite as an electron acceptor. They require a minimum "anoxic SRT " (similar in concept to the minimum aerobic SRT required by autotrophs) to maintain themselves in the activated sludge system without washing out. Nitrogen source for cell synthesis of these microorganisms is ammonia. The base rate expression for this growth process is the product of the maximum specific growth rate, the anoxic methylotrophs concentration and a Monod expression for methanol. This base rate is modified to account for environmental conditions (dissolved oxygen, nitrate and nitrite), nutrient limitations (ammonia, phosphate, other cations and anions), pH inhibition and electron acceptor preference weighting. BioWin preferentially uses nitrite as an electron acceptor.

The single decay rate varies between an aerobic value and an unaerated value depending oxygen concentration.

Model parameters are listed in:

### *Kinetic Parameters*

Menu Location: **Project|Parameters|Kinetic|Methylotrophs**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Max. spec. growth rate of methanol | 1.3 | $d^{-1}$ | Determines the maximum specific growth rate of methylotrophs. |

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| utilizers | | | Substrate and nutrient limitations will decrease the growth rate. This parameter will determine the necessary anoxic SRT to maintain a viable denitrifying population on methanol. |
| Methanol half sat. | 0.5 | mgCOD/L | This parameter impacts the residual methanol concentration bleeding out of the anoxic tank. The value is usually very low in normal municipal plants (once the suitable population has been established). |
| Aerobic decay rate of methanol utilizers | 0.04 | $d^{-1}$ | Decay rate constant under aerobic conditions. This parameter impacts the minimum anoxic SRT. |
| Anoxic/anaerobic decay rate of methanol utilizers | 0.03 | $d^{-1}$ | Decay rate constant in the absence of oxygen. This parameter impacts the minimum anoxic SRT. |

## *Stoichiometric Parameters*

Menu Location: **Project|Parameters|Stoichiometric|Methylotrophs**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Yield (anoxic) | 0.4 | mgCOD/mgCOD | Anoxic methylotrophic biomass yield on readily methanol COD under anoxic conditions. This parameter has significant impact on the methanol dosage required to denitrify 1 mgN nitrate (3.2mg methanol/mg$NO_3$-N by default) |
| N in Biomass | 0.07 | mgN/ mgCOD | N content of anoxic methylotrophs. |
| N in Inert | 0.07 | mgN/ mgCOD | N content of endogenous residue from anoxic methylotrophic organism decay. |
| P in Biomass | 0.022 | mgP/ mgCOD | P content of anoxic methylotrophs. |
| P in Inert | 0.022 | mgP/ mgCOD | P content of endogenous residue from anoxic methylotrophic organism decay. |
| Endogenous Residue | 0.08 | - | Fraction of biomass that becomes inert upon decay. |
| COD:VSS Ratio | 1.42 | mgCOD/mgVSS | Conversion factor between biomass as measured in COD and its VSS content. This value is relatively stable for biomass. |

## *pH Inhibition*

Menu Location: **Project|Parameters|Kinetic|pH**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| √Methanol tilizers low pH limit | 4.0 | pH units | At a pH equal to this value the growth rate of methylotrophs will be reduced by 50%. |
| Methanol utilizers high pH limit | 10.0 | pH units | At a pH equal to this value the growth rate of methylotrophs will be reduced by 50%. |

### *Switching Functions*

Menu Location: **Project|Parameters|Kinetic|Switches**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Heterotrophic DO half sat. | 0.05 | $mgO_2/L$ | This constant is used to switch off aerobic activity under low DO conditions (that is in anaerobic and anoxic reactors). |
| Anoxic NO3 half sat. | 0.1 | mgN/L | This constant is used to switch off anoxic growth processes using nitrate under low nitrate conditions. |
| Anoxic NO2 half sat. | 0.1 | mgN/L | This constant is used to switch off anoxic growth processes using nitrite under low nitrite conditions. |
| NH3 nutrient half sat. | 0.001 | mgN/L | This constant is used to slow all biomass growth processes at low ammonia-N concentrations (N nutrient limiting conditions – see assimilative denitrification). |
| P nutrient half sat. | 0.001 | mgP/L | This constant is used to slow the growth of biomass when there is no phosphorus available as nutrient. |
| Synthesis anion/cation half sat. | 0.01 | meq/L | Half saturation concentration for anions and cations. |

## Hydrolysis, Adsorption, Ammonification and Assimilative denitrification

**Number of Processes:** 7

**Engineering Objective:** Conversion of organic, nitrogen and phosphorus fractions

**Implementation:** permanent, always active in the BioWin model

**Module Description:**

These processes are discussed here separately from the organism groupings because they involve more that one organism type (in general both the ordinary heterotrophic organisms and the phosphate accumulating organisms.

**Hydrolysis of biodegradable particulate organic substrate to readily biodegradable complex substrate**: The base rate is the product of the hydrolysis rate constant, the sum of the ordinary heterotrophs and the phosphate accumulating organisms, and a Monod expression for ratio of particulate substrate to organism COD. There is an efficiency factor applied for anoxic conditions and another for anaerobic conditions.

**Hydrolysis of biodegradable particulate organic nitrogen and phosphorus:** The hydrolysis of biodegradable particulate nitrogen (phosphorus) is assumed to proceed at the same rate as the biodegradable particulate organics but is adjusted by the ratio of biodegradable particulate organic nitrogen (phosphorus) to biodegradable particulate organic.

**Adsorption or flocculation of colloidal organic material to particulate organic material (occurring spontaneously as opposed to chemically facilitated flocculation with metal (ferric or alum) addition:** The rate is the product of the adsorption rate constant, the colloidal substrate concentration and the sum of the ordinary heterotrophs and the phosphate accumulating organism concentrations. The rate is decreased as the ratio of particulate substrate to organism COD approaches the maximum adsorption ratio constant.

**Ammonification of soluble organic nitrogen to ammonia:** The rate is the product of the ammonification rate constant, the soluble organic nitrogen concentration and the sum of the ordinary heterotrophs and the phosphate accumulating organism concentrations.

**Assimilative denitrification of nitrate or nitrite to ammonia for synthesis:** BioWin allows for the production of ammonia for synthesis by any organisms under low ammonia conditions (as ammonia becomes limiting for growth). The assimilative process will use nitrite if it is available otherwise it will use nitrate. The base rate is the product of the assimilation rate constant and the total organism COD. This base rate is modified to account for environmental conditions (off with ammonia, and selecting between nitrate and nitrite).

Model parameters are listed in:

## *Kinetic Parameters*

Menu Location: **Project|Parameters|Kinetic|OHOs**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Hydrolysis rate (AS) | 2.1 | $d^{-1}$ | Rate constant for hydrolysis of slowly degradable organics into readily degradable substrate; for activated sludge. |
| Hydrolysis half sat. (AS) | 0.06 | - | Monod half saturation constant for the regulation of hydrolysis rate, expressed in terms of particulate substrate to heterotrophic biomass ratio; for activated sludge. |
| Anoxic hydrolysis factor | 0.28 | - | Rate reduction factor for hydrolysis under anoxic conditions. |
| Anaerobic hydrolysis factor | 0.5 | - | Rate reduction factor for hydrolysis under anaerobic conditions in activated sludge. |
| Adsorption rate of colloids | 0.8 | $d^{-1}$ | Conversion rate of colloidal material to particulate. |

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|---|---|---|---|
| Ammonification rate | 0.04 | $d^{-1}$ | Conversion rate of soluble organic nitrogen compounds to ammonia |
| Assimilative nitrate/nitrite reduction rate | 0.5 | $d^{-1}$ | Conversion rate of nitrite and/or nitrate to ammonia under ammonia limited conditions |
| Hydrolysis rate (AD) | 0.1 | $d^{-1}$ | Hydrolysis rate of particulate organics in anaerobic digesters |
| Hydrolysis half sat. (AD) | 0.15 | - | Monod half saturation constant for regulation of hydrolysis rate in anaerobic digesters, expressed in terms of particulate substrate to heterotrophic biomass ratio |

### *Stoichiometric Parameters*

**None**

### *Switching Functions*

Menu Location: **Project|Parameters|Kinetic|Switches**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Heterotrophic DO half sat. | 0.05 | $mgO_2/L$ | This constant is used to switch off aerobic activity under low DO conditions (that is in anaerobic and anoxic reactors). |
| Anoxic NO3 half sat. | 0.1 | mgN/L | This constant is used to switch off anoxic growth processes using nitrate under low nitrate conditions. |
| Anoxic NO2 half sat. | 0.1 | mgN/L | This constant is used to switch off anoxic growth processes using nitrite under low nitrite conditions. |
| NH3 nutrient half sat. | 0.001 | mgN/L | This constant is used to slow all biomass growth processes at low ammonia-N concentrations (N nutrient limiting conditions – see assimilative denitrification**).** |

## Growth and Decay of Ammonia Oxidizing Biomass (AOB)

**Number of Processes:** 2

**Engineering Objective:** Nitrification

**Implementation:** permanent, always active in the BioWin model

**Module Description:**

This biomass grows by oxidizing ammonia to nitrite and using the energy to synthesis organic material from inorganic carbon (fixing $CO_2$). Nitrogen source for cell synthesis is ammonia.

The base rate expression for the growth process is the product of the maximum specific growth rate, the ammonia oxidizing biomass concentration and a Monod expression for ammonia. This base rate is modified to account for environmental conditions (off at low dissolved oxygen and inhibited by nitrous acid), nutrient limitations (phosphate, inorganic carbon, other cations and anions) and pH inhibition.

The decay rate varies between an aerobic value and an anoxic/anaerobic value depending dissolved oxygen concentrations.

Model parameters are listed in:

## *Kinetic Parameters*

Menu Location: **Project|Parameters|Kinetic|AOB**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Max. spec. growth rate | 0.9 | d-1 | Determines the maximum specific growth rate of ammonia oxidizing biomass. Substrate and nutrient limitations will decrease the growth rate. This parameter has a direct impact on the nitrification capacity. |
| Substrate ($NH_4$) half sat. | 0.7 | mgN/L | This parameter impacts the residual ammonia concentration in the effluent. The value is usually low in normal municipal plants. |
| Aerobic decay rate | 0.17 | d-1 | Decay rate constant under aerobic conditions for ammonia oxidizing biomass. |
| Anoxic/anaerobic decay rate | 0.08 | d-1 | Decay rate constant under non-aerobic conditions for ammonia oxidizing biomass. |
| $KiHNO_2$ | 0.005 | mmol/L | Nitrous acid inhibition concentration. |

## *Stoichiometric Parameters*

Menu Location: **Project|Parameters|Stoichiometric|AOB**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Yield | 0.15 | mgCOD/mgN | AOB COD produced by oxidizing 1 mg of ammonia. |
| N in biomass | 0.07 | mgN/ mgCOD | N content of AOB. |
| N in inert | 0.07 | mgN/ mgCOD | N content of endogenous residue from AOB decay. |
| P in biomass | 0.022 | mgP/ mgCOD | P content of AOB. |
| P in inert | 0.022 | mgP/ mgCOD | P content of endogenous residue from AOB decay. |
| Fraction to endogenous | 0.08 | - | Fraction of biomass that becomes inert upon decay. |

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| residue | | | |
| COD:VSS ratio | 1.42 | mgCOD/mgVSS | Conversion factor between biomass as measured in COD and its VSS content. This value is relatively stable for biomass. |

### *pH Inhibition*

Menu Location: **Project|Parameters|Kinetic|pH**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Autotrophs low pH limit | 5.5 | pH units | At a pH equal to this value the growth rate of AOB, NOB and ANAMMOX will be reduced by 50%. |
| Autotrophs high pH limit | 9.5 | pH units | At a pH equal to this value the growth rate of AOB, NOB and ANAMMOX will be reduced by 50%. |

### *Switching Functions*

Menu Location: **Project|Parameters|Kinetic|Switches**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Ammonia oxidizer DO half sat. | 0.25 | $mgO_2/L$ | This parameter is used to switch off ammonia oxidation by AOB under low DO conditions. |
| P nutrient half sat. | 0.001 | mgP/L | This parameter is used to switch off the growth of biomass when there is no phosphorus available as nutrient. |
| Autotroph CO2 half sat. | 0.1 | mmol/L | This parameter is used to switch off the growth of AOB, NOB and ANAMMOX when there is little inorganic carbon available. |
| Synthesis anion/cation half sat. | 0.01 | meq/L | Half saturation concentration for anions and cations. |

## Growth and Decay of Nitrite Oxidizing Biomass (NOB)

**Number of Processes:** 2

**Engineering Objective:** Nitrification

**Implementation:** permanent, always active in the BioWin model

**Module Description:**

This biomass grows by oxidizing nitrite to nitrate and using the energy to synthesis organic material from inorganic carbon (fixing $CO_2$). Nitrogen source for cell synthesis is ammonia.

The base rate expression for the growth process is the product of the maximum specific growth rate, the nitrite oxidizing biomass concentration and a Monod expression for nitrite. This base rate is modified to account for environmental conditions (off at low dissolved oxygen and inhibited by ammonia), nutrient limitations (ammonia, phosphate, inorganic carbon, other cations and anions) and pH inhibition.

The decay rate varies between an aerobic value and an anoxic/anaerobic value depending dissolved oxygen concentrations.

Model parameters are listed in:

### *Kinetic Parameters*

Menu Location: **Project|Parameters|Kinetic|NOB**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Max. spec. growth rate | 0.7 | d-1 | Determines the maximum specific growth rate of nitrite oxidizing biomass. Substrate, nutrient limitations and environmental conditions will decrease the growth rate. This parameter has a direct impact on the nitrification capacity. |
| Substrate ($NO_2$) half sat. | 0.05 | mgN/L | This parameter impacts the residual nitrite concentration in the effluent. The value is usually very low in normal municipal plants. |
| Aerobic decay rate | 0.17 | d-1 | Decay rate constant under aerobic conditions for nitrite oxidizing biomass. |
| Anoxic/anaerobic decay rate | 0.08 | d-1 | Decay rate constant under non-aerobic conditions for nitrite oxidizing biomass. |
| $KiHNH_3$ | 0.075 | mmol/L | NH3 inhibition concentration. |

### *Stoichiometric Parameters*

Menu Location: **Project|Parameters|Stoichiometric|NOB**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Yield | 0.09 | mgCOD/mgN | NOB COD produced by oxidizing 1 mg of nitrite N. |
| N in biomass | 0.07 | mgN/ mgCOD | N content of NOB. |
| N in inert | 0.07 | mgN/ mgCOD | N content of endogenous residue from NOB decay. |
| P in biomass | 0.022 | mgP/ mgCOD | P content of NOB. |
| P in inert | 0.022 | mgP/ mgCOD | P content of endogenous residue from NOB decay. |

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| Fraction to endogenous residue | 0.08 | - | Fraction of biomass that becomes inert upon decay. |
| COD:VSS ratio | 1.42 | mgCOD/mgVSS | Conversion factor between biomass as measured in COD and its VSS content. This value is relatively stable for biomass. |

### *pH Inhibition*

Menu Location: **Project|Parameters|Kinetic|pH**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Autotrophs low pH limit | 5.5 | pH units | At a pH equal to this value the growth rate of AOB, NOB and ANAMMOX will be reduced by 50%. |
| Autotrophs high pH limit | 9.5 | pH units | At a pH equal to this value the growth rate of AOB, NOB and ANAMMOX will be reduced by 50%. |

### *Switching Functions*

Menu Location: **Project|Parameters|Kinetic|Switches**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Nitrite oxidizer DO half sat. | 0.5 | $mgO_2/L$ | This parameter is used to switch off nitrite oxidation by NOB under low DO conditions. |
| P nutrient half sat. | 0.001 | mgP/L | This parameter is used to switch off the growth of biomass when there is no phosphorus available as nutrient. |
| Autotroph CO2 half sat. | 0.1 | mmol/L | This parameter is used to switch off the growth of AOB, NOB and ANAMMOX when there is little inorganic carbon available. |
| Synthesis anion/cation half sat. | 0.01 | meq/L | Half saturation concentration for anions and cations. |

## Growth and Decay of ANaerobic AMMonia OXidizers (ANAMMOX)

**Number of Processes:** 2

**Engineering Objective:** Nitrification

**Implementation:** permanent, always active in the BioWin model

**Module Description:**

This biomass grows by converting ammonia and nitrite to nitrogen gas and nitrate. The energy from this process is used to synthesis organic material from inorganic carbon (fixing $CO_2$). Nitrogen source for cell synthesis is ammonia.

The base rate expression for the growth process is the product of the maximum specific growth rate, the ANAMMOX concentration, a Monod expression for ammonia and a Monod expression for nitrite. This base rate is modified to account for environmental conditions (switched off under aerobic conditions and inhibited by nitrite), nutrient limitations (phosphate, inorganic carbon, other cations and anions) and pH inhibition.

The decay rate varies between an aerobic and anoxic/anaerobic value depending dissolved oxygen concentrations. Nitrite toxicity is modeled by increasing the decay rate by the product of the nitrite sensitivity constant and the nitrite concentration.

Model parameters are listed in:

### *Kinetic Parameters*

Menu Location: **Project|Parameters|Kinetic|ANAMMOX**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Max. spec. growth rate | 0.1 | d-1 | Determines the maximum specific growth rate of ANAMMOX. Substrate, nutrient limitations and environmental conditions will decrease the growth rate. This parameter has a direct impact on the nitrification capacity. |
| Substrate ($NH_4$) half sat. | 2.0 | mgN/L | Ammonia half saturation concentration for ANNAMOX. |
| Substrate ($NO_2$) half sat. | 1.0 | mgN/L | Nitrite half saturation concentration for ANNAMOX. |
| Aerobic decay rate | 0.019 | d-1 | Decay rate constant under aerobic conditions for ANNAMOX. |
| Anoxic/anaerobic decay rate | 0.0095 | d-1 | Decay rate constant under non-aerobic conditions for ANNAMOX. |
| Ki Nitrite | 1000.0 | mgN/L | Nitrite inhibition concentration. |
| Nitrite sensitivity constant | 0.016 | L/ (d mgN) | Nitrite toxicity constant. |

### *Stoichiometric Parameters*

Menu Location: **Project|Parameters|Stoichiometric|ANNAMOX**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Yield | 0.114 | mgCOD/mgN | ANNAMOX produced by oxidizing 1 mg of ammonia. |
| Nitrate production | 2.28 | mgN/mgCOD | Nitrate production yield |
| N in biomass | 0.07 | mgN/ mgCOD | N content of ANNAMOX. |

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|---|---|---|---|
| N in inert | 0.07 | mgN/ mgCOD | N content of endogenous residue from ANNAMOX decay. |
| P in biomass | 0.022 | mgP/ mgCOD | P content of ANNAMOX. |
| P in inert | 0.022 | mgP/ mgCOD | P content of endogenous residue from ANNAMOX decay. |
| Fraction to endogenous residue | 0.08 | - | Fraction of biomass that becomes inert upon decay. |
| COD:VSS ratio | 1.42 | mgCOD/mgVSS | Conversion factor between biomass as measured in COD and its VSS content. This value is relatively stable for biomass. |

### *pH Inhibition*

Menu Location: **Project|Parameters|Kinetic|pH**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Autotrophs low pH limit | 5.5 | pH units | At a pH equal to this value the growth rate of AOB, NOB and ANAMMOX will be reduced by 50%. |
| Autotrophs high pH limit | 9.5 | pH units | At a pH equal to this value the growth rate of AOB, NOB and ANAMMOX will be reduced by 50%. |

### *Switching Functions*

Menu Location: **Project|Parameters|Kinetic|Switches**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Anaerobic ammonia oxidizer DO half sat. | 0.01 | $mgO_2/L$ | This parameter is used to switch on anaerobic ammonia oxidation by ANNAMOX under very low DO conditions. |
| P nutrient half sat. | 0.001 | mgP/L | This parameter is used to switch off the growth of biomass when there is no phosphorus available as nutrient. |
| Autotroph CO2 half sat. | 0.1 | mmol/L | This parameter is used to switch off the growth of AOB, NOB and ANAMMOX when there is little inorganic carbon available. |
| Synthesis anion/cation half sat. | 0.01 | meq/L | Half saturation concentration for anions and cations. |

# Growth and Decay of Phosphorus Accumulating Organisms

**Number of Processes:** 15

**Engineering Objective:** Biological phosphorus removal

**Implementation:** permanent, always active in the BioWin model

**Module Description:**

This group of processes describes the growth and decay of polyphosphate accumulating organisms (PAOs) under all conditions. This includes descriptions of aerobic and anoxic growth, VFA sequestration and polyphosphate lysis.

There are two maximum specific growth rates for PAOs under aerobic conditions. The lower growth rate constant is used under P limited conditions and has a different stoichiometry (no polyphosphate storage). There are also two anoxic growth processes, one uses nitrate and the other nitrite. Growth processes under phosphate rich conditions result in uptake of phosphate, and balancing calcium magnesium ions and other cations. A lack of these ions will stop the growth processes by appropriate Monod switches. For all of these growth processes, the base growth rate is the product of the maximum specific rate constant, the PAO concentration and a Monod on the ratio PAO COD to PHA COD. This base rate is modified to account for environmental conditions (dissolved oxygen, nitrate and nitrite), nutrient limitations (ammonia, anions, cations, for polyphosphate storage magnesium, and calcium are also required) and pH inhibition. BioWin uses ammonia as a nitrogen source for cell synthesis under aerobic, anoxic and anaerobic conditions. At low ammonia concentrations BioWin allows for assimilative ammonia production from either nitrate or nitrite in order to satisfy synthesis demands.

Under anoxic conditions the base rate is also multiplied by an anoxic growth factor and preferentially uses nitrite as the electron acceptor.

The PAOs use energy store in polyphosphate to sequester acids and store them as store PHA. In the BioWin model the PAOs can use both acetate and propionate for this process. The base sequestration rate is the product of the sequestration rate constant, the PAO concentration and a Monod on the appropriate substrate (acetate or propionate) The base rate is switched on the availability of the stored polyphosphate (ratio of low molecular weight polyphosphate to PAO COD).

There are two decay processes (aerobic and anoxic/anaerobic). Associated with each decay process is a lysis process for PHA, low and high molecular weight polyphosphate. The lysis rates are directly proportional to the decay rate itself.

There is one Poly-P cleavage process for anaerobic maintenance that releases phosphate if no oxygen is present. This process is proportional to the anoxic/anaerobic decay rate.

Model parameters are listed in:

## *Kinetic Parameters*

Menu Location: **Project|Parameters|Kinetic|PAOs**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Max. spec. growth rate | 0.95 | $d^{-1}$ | Determines the maximum attainable growth rate of phosphorus accumulating heterotrophic |

| | | | |
|---|---|---|---|
| | | | organisms if no substrate, DO or P limitation occurs. |
| Max. spec. growth rate, P-limited | 0.42 | $d^{-1}$ | Determines the maximum attainable growth rate of phosphorus accumulating heterotrophic organisms under phosphorus limiting conditions. |
| Substrate half sat. | 0.1 | mgCOD/L | Half saturation constant for PHA, used as substrate by phosphorus accumulating organisms. |
| Substrate half sat., P-limited | 0.05 | mgCOD/L | Half saturation constant for PHA, under phosphorus limiting conditions. |
| Magnesium half sat. | 0.1 | mgMg/L | Half saturation constant for Magnesium storage during poly-P synthesis. |
| Cation half sat. | 0.1 | meq/L | Half saturation constant for cation (primarily potassium) storage during poly-P synthesis. |
| Aerobic decay rate | 0.1 | $d^{-1}$ | Decay rate constant in aerobic conditions. |
| Anaerobic decay rate | 0.04 | $d^{-1}$ | Decay rate constant when there is no oxygen available. |
| Sequestration rate | 6.0 | $d^{-1}$ | Rate constant for VFA sequestration to form PHA (stored substrate). |
| Anoxic growth factor | 0.33 | - | Together with the max. spec. growth rate, determines the maximum attainable growth rate if nitrate is available only as electron acceptor (and no substrate limitation occurs). |

## *Stoichiometric Parameters*

Menu Location: **Project|Parameters|Stoichiometric|PAOs**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Yield (aerobic) | 0.639 | mgCOD/mgCOD | Amount of biomass produced using one unit of substrate under aerobic conditions. The rest of the substrate will be oxidized. |
| Yield (anoxic) | 0.52 | mgCOD/mgCOD | Amount of biomass produced using one unit of substrate under anoxic conditions. |
| Aerobic P/PHA uptake | 0.95 | mgP/mgCOD | Amount of P stored per unit of PHA oxidized in aerobic conditions |
| Anoxic P/PHA uptake | 0.35 | mgP/mgCOD | Amount of P stored per unit of PHA in anoxic conditions. |
| Yield of PHA on sequestration | 0.889 | mgCOD/mgCOD | Amount of PHA stored when 1 mg of acetate or propionate is sequestered. |
| N in biomass | 0.07 | mgN/ mgCOD | N content of phosphorus accumulating organisms. Has a significant effect on nitrogen availability for nitrification and |

| | | | |
|---|---|---|---|
| | | | therefore oxygen demand. |
| N in part. inert | 0.07 | mgN/ mgCOD | N content of endogenous residue originating from phosphorus accumulating organism decay. |
| N in sol. inert | 0.07 | mgN/ mgCOD | N content of soluble inert organics originating from phosphorus accumulating organism decay. |
| P in biomass | 0.022 | mgP/ mgCOD | P content of phosphorus accumulating organisms, not including P stored in the form of Poly-P |
| P in part. inert | 0.022 | mgP/ mgCOD | P content of endogenous residue originating from phosphorus accumulating organism decay. |
| Fraction to inert part. | 0.25 | - | Fraction of biomass that becomes particulate inert upon decay. |
| Fraction to inert sol. | 0.2 | - | Fraction of biomass that becomes soluble inert upon decay. |
| P/Ac release ratio | 0.49 | mgP/mgCOD | Amount of P released for one mg of acetate sequestered in the form of PHA |
| COD:VSS Ratio | 1.42 | mgCOD/mgVSS | Conversion factor between biomass as measured in COD and its VSS content. This value is relatively stable for biomass. |
| Yield of low PP | 0.94 | mgP/mgP | Fraction of P stored in releasable poly-P form (rest of P is stored in high molecular weight, non-releasable poly-P) |

## *pH Inhibition*

Menu Location: **Project|Parameters|Kinetic|pH**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| PolyP heterotrophs low pH limit | 4.0 | pH units | At a pH equal to this value the growth rate of poly phosphate accumulating biomass will be reduced by 50%. |
| Poly P heterotrophs high pH limit | 10.0 | pH units | At a pH equal to this value the growth rate of poly phosphate accumulating biomass will be reduced by 50%. |

## *Switching Functions*

Menu Location: **Project|Parameters|Kinetic|Switches**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Heterotrophic | 0.05 | $mgO_2/L$ | This constant is used to switch off aerobic |

| | | | |
|---|---|---|---|
| DO half sat. | | | OHO activity under low DO conditions (that is in anaerobic and anoxic reactors). |
| Anoxic NO3 half sat. | 0.1 | mgN/L | This constant is used to switch off anoxic growth processes using nitrate under low nitrate conditions. |
| Anoxic NO2 half sat. | 0.1 | mgN/L | This constant is used to switch off anoxic growth processes using nitrite under low nitrite conditions. |
| NH3 nutrient half sat. | 0.001 | mgN/L | This constant is used to slow all biomass growth processes at low ammonia-N concentrations (N nutrient limiting conditions – see assimilative denitrification). |
| PolyP half sat. | 0.01 | mgP/L | This constant stops sequestration of VFA and P release as the ratio of low molecular weight polyphosphate to PAO COD falls. |
| VFA sequestration half sat. | 5.0 | mgCOD/L | This is the half saturation concentration for the sequestration of acetate and propionate. |
| P uptake half sat. | 0.15 | mgP/L | This constant stops growth with poly phosphate storeage at low soluble phosphate concentrations. This constant will have an impact on the effluent soluble P concentration in a bio-P system. |
| P nutrient half sat. | 0.001 | mgP/L | This constant is used to slow the growth of biomass when there is no phosphorus available as nutrient. |
| Synthesis anion/cation half sat. | 0.01 | meq/L | Half saturation concentration for anions and cations. |

## *Other Parameters*

Menu Location: **Project|Parameters|Other|General**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Mg to P mole ratio in polyphosphate | 0.3 | molMg/molP | Mole ratio of magnesium to phosphorus in stored polyphosphate. This magnesium is released when polyphosphate is used (together with the phosphate release). |
| Cation to P mole ratio in polyphosphate | 0.3 | meq/mmolP | Mole ratio of other cations (primarily potassium) to phosphorus in stored polyphosphate. These cations are released when polyphosphate is used (together with the phosphate release). |
| Ca to P mole ratio in polyphosphate | 0.05 | molCa/molP | Mole ratio of calcium to phosphorus in stored polyphosphate. This calcium is released when polyphosphate is used (together with the phosphate release). |

# Anaerobic Digestion Model

The anaerobic digestion model in BioWin contains the following functional categories, modules

**Heterotrophic Growth through Fermentation**

**Growth and Decay of Propionic Acetogens**

**Growth and Decay of Methanogens**

These modules are described in detail below.

## Heterotrophic Growth through Fermentation

**Number of Processes:** 2

**Engineering Objective:** VFA generation (fermenters, digesters)

**Implementation:** permanent, always active in the BioWin model

**Module Description:**

There are two pathways for the fermentation of readily biodegradable (complex) substrate to acetate, propionate, carbon dioxide and hydrogen. The dominant pathway is governed by the dissolved hydrogen concentration. These processes are mediated by the ordinary heterotrophic organisms.

The base rate expression for the fermentation growth process is the product of the maximum specific growth rate constant, the heterotrophic biomass concentration and a Monod expression for the readily biodegradable (complex) substrate. This base rate is modified to account for nutrient limitations (ammonia, phosphate, other cations and anions) and pH inhibition. In activated sludge vessels there is an anaerobic growth factor applied. BioWin uses ammonia as a nitrogen source for cell synthesis.

Model parameters affecting the performance of this module are listed below.

### *Kinetic Parameters*

Menu Location: **Project|Parameters|Kinetic|OHOs**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Anoxic/anaerobic decay* | 0.3 | $d^{-1}$ | Decay rate constant when there is no oxygen available. |
| Fermentation rate | 3.2 | $d^{-1}$ | Maximum specific growth rate of heterotrophs under anaerobic conditions. |
| Fermentation half sat. | 5.0 | mgCOD/L | Half saturation of complex substrate under anaerobic conditions |
| Anaerobic growth factor (AS) | 0.125 | - | Growth rate reduction under anaerobic conditions in activated sludge |

### *Stoichiometric Parameters*

Menu Location: **Project|Parameters|Stoichiometric|OHOs**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Yield (fermentation low H2) | 0.1 | mgCOD/mgCOD | Amount of biomass produced on one unit of complex substrate fermented, under low $H_2$ concentration. |
| Yield (fermentation high H2) | 0.1 | mgCOD/mgCOD | Amount of biomass produced on one unit of complex substrate fermented, under high $H_2$ concentration. |
| H2 yield (fermentation low H2) | 0.35 | mgCOD/mgCOD | Amount of hydrogen produced on one unit of complex substrate fermented, under low $H_2$ concentration. |
| H2 yield (fermentation high H2) | 0.0 | mgCOD/mgCOD | Amount of hydrogen produced on one unit of complex substrate fermented, under high $H_2$ concentration. |
| Propionate yield (fermentation low H2) | 0.0 | mgCOD/mgCOD | Amount of propionate produced on one unit of complex substrate fermented, under low $H_2$ concentration. |
| Propionate yield (fermentation high H2) | 0.7 | mgCOD/mgCOD | Amount of propionate produced on one unit of complex substrate fermented, under high $H_2$ concentration. |
| CO2 yield (fermentation low H2) | 0.7 | mmol$CO_2$/mmolHAC | Moles of $CO_2$ produced per mole of acetate formed at low dissolved $H_2$ concentrations. |
| CO2 yield (fermentation high H2) | 0.0 | mmol$CO_2$/mmolHAC | Moles of $CO_2$ produced per mole of acetate formed at high dissolved $H_2$ concentrations. |
| N in Biomass | 0.07 | mgN/ mgCOD | N content of biomass. |
| N in Inert | 0.07 | mgN/ mgCOD | N content of endogenous residue originating from heterotrophic decay. |
| P in Biomass | 0.022 | mgP/ mgCOD | P content of heterotrophs. This parameter influences the P removal in non bio-P systems, and the P content of the sludge. |
| P in Inert | 0.022 | mgP/ mgCOD | P content of endogenous residue originating from heterotrophic decay. |
| Endogenous Residue | 0.08 | - | Fraction of biomass that becomes inert upon decay. |
| COD:VSS Ratio | 1.42 | mgCOD/mgVSS | Conversion factor between biomass as measured in COD and its VSS content. This value is relatively stable for biomass. |

### *pH Inhibition*

Menu Location: **Project|Parameters|Kinetic|pH**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Heterotrophs low pH limit (anaerobic) | 5.5 | pH units | At a pH equal to this value the growth rate of ordinary heterotrophic biomass in an anaerobic will be reduced by 50%. |
| Heterotrophs high pH limit (anaerobic) | 8.5 | pH units | At a pH equal to this value the growth rate of ordinary heterotrophic biomass in an anaerobic will be reduced by 50%. |

### *Switching Functions*

Menu Location: **Project|Parameters|Kinetic|Switches**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Heterotrophic DO half sat. | 0.05 | $mgO_2/L$ | This constant is used to switch off aerobic OHO activity under low DO conditions (that is in anaerobic and anoxic reactors). |
| Anoxic NO3 half sat. | 0.1 | mgN/L | This constant is used to switch off anoxic growth processes using nitrate under low nitrate conditions. |
| Anoxic NO2 half sat. | 0.1 | mgN/L | This constant is used to switch off anoxic growth processes using nitrite under low nitrite conditions. |
| NH3 nutrient half sat. | 0.001 | mgN/L | This constant is used to slow all biomass growth processes at low ammonia-N concentrations (N nutrient limiting. |
| P nutrient half sat. | 0.001 | mgP/L | This constant is used to slow the growth of biomass when there is no phosphorus available as nutrient. |
| Heterotrophic Hydrogen half sat. | 1.0 | mgCOD/L | This constant switches between two fermentation pathways, generating acetate and propionate in various ratios, depending on available $H_2$ concentration. |
| Synthesis anion/cation half sat. | 0.01 | meq/L | Half saturation concentration for anions and cations. |

## Growth and Decay of Propionic Acetogens

**Number of Processes:** 2

**Engineering Objective:** anaerobic digestion

**Implementation:** permanent, always active in the BioWin model

**Module Description:**

These 2 processes describe the growth and decay of propionic acetogens, converting propionate to acetate, $CO_2$ and hydrogen. Nitrogen source for cell synthesis is ammonia. The base rate expression the growth process is the product of the maximum specific growth rate, the propionic acetogen biomass concentration and a Monod expression for propionate. This base rate is modified to account for environmental conditions (off unless anaerobic, inhibited by hydrogen and acetate), nutrient limitations (nitrogen, phosphate, other cations and anions) and pH inhibition. BioWin uses ammonia as a nitrogen source for cell synthesis.

The decay process has a rate that varies according to the electron acceptor environment

Model parameters are listed in:

## *Kinetic Parameters*

Menu Location: **Project|Parameters|Kinetic|Acetogens**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Max. spec. growth rate | 0.25 | $d^{-1}$ | Maximum specific growth rate in the absence of substrate limitations. |
| Substrate half sat. | 10.0 | mgCOD/L | Half saturation for regulation of growth rate, based on availability of propionate as substrate |
| Acetate inhibition | 10000 | mgCOD/L | Acetate inhibition constant: high acetate concentrations inhibit propionic acetogen growth. |
| Decay rate | 0.05 | $d^{-1}$ | Decay rate constant when there is no oxygen available. |
| Aerobic decay rate | 0.52 | $d^{-1}$ | Decay rate constant in the presence of oxygen. |

## *Stoichiometric*

Menu Location: **Project|Parameters|Stoichiometric|Acetogens**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Yield | 0.1 | mgCOD/mgCOD | Amount of biomass produced on one unit of propionate converted. |
| H2 yield | 0.4 | mgCOD/mgCOD | Amount of $H_2$ produced on one unit of propionate converted. |
| CO2 yield | 1.0 | mmol$CO_2$/mmol | Moles of $CO_2$ produced per mole |
| N in biomass | 0.07 | mgN/ mgCOD | N content of propionic acetogens. |
| N in endogenous | 0.07 | mgN/ mgCOD | N content of endogenous residue originating from |

| | | | |
|---|---|---|---|
| residue | | | propionic acetogen decay. |
| P in biomass | 0.022 | mgP/ mgCOD | P content of propionic acetogens. |
| P in endogenous residue | 0.022 | mgP/ mgCOD | P content of endogenous residue originating from propionic acetogen decay. |
| Fraction to endogenous residue | 0.08 | - | Fraction of biomass that becomes inert upon decay. |
| COD:VSS ratio | 1.42 | mgVSS/mgCOD | Conversion factor between biomass as measured in COD and its VSS content. This value is relatively stable for biomass. |

### *pH Inhibition*

Menu Location: **Project|Parameters|Kinetic|pH**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Propionic acetogens low pH limit | 4.0 | pH units | At a pH equal to this value the growth rate of propionic acetogens will be reduced by 50%. |
| Propionic acetogens high pH limit | 10.0 | pH units | At a pH equal to this value the growth rate of propionic acetogens will be reduced by 50%. |

### *Switching Functions*

Menu Location: **Project|Parameters|Kinetic|Switches**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Heterotrophic DO half sat. | 0.05 | $mgO_2/L$ | This constant is used to switch off aerobic OHO activity under low DO conditions (that is in anaerobic and anoxic reactors). |
| Anoxic NO3 half sat. | 0.1 | mgN/L | This constant is used to switch off anoxic growth processes using nitrate under low nitrate conditions. |
| Anoxic NO2 half sat. | 0.1 | mgN/L | This constant is used to switch off anoxic growth processes using nitrite under low nitrite conditions. |
| NH3 nutrient half sat. | 0.001 | mgN/L | This constant is used to slow all biomass growth processes at low ammonia-N concentrations (N nutrient limiting. |
| P nutrient half sat. | 0.001 | mgP/L | This constant is used to slow the growth of biomass when there is no phosphorus |

| | | | |
|---|---|---|---|
| | | | available as nutrient. |
| Propionic acetogens Hydrogen limit | 5.0 | mgCOD/L | This constant is used to inhibit the growth of biomass when high levels of $H_2$ are present. |
| Synthesis anion/cation half sat. | 0.01 | meq/L | Half saturation concentration for anions and cations. |

## Growth and Decay of Methanogens

**Number of Processes:** 6

**Engineering Objective:** anaerobic digestion

**Implementation:** permanent, always active in the BioWin model

**Module Description:**

These 6 processes describe the growth and decay of two of the principal groups of obligate anaerobic microorganisms (acetoclastic methanogens converting acetate (or methanol) to methane and $CO_2$; and hydrogenotrophic methanogens, converting $CO_2$ (or methanol) and hydrogen to methane and water).

The base rate expression for each of the 4 growth processes is the product of the maximum specific growth rate constant, the appropriate biomass concentration and a Monod expression for each of the substrates. This base rate is modified to account for nutrient limitations (ammonia, phosphate, other cations and anions) and pH inhibition. BioWin uses ammonia as a nitrogen source for cell synthesis

For both populations, the decay rate that varies according to the electron acceptor environment.

Model parameters are listed in:

### *Kinetic Parameters*

Menu Location: **Project|Parameters|Kinetic|Methanogens**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Acetoclastic Mu Max | 0.3 | $d^{-1}$ | Maximum specific growth rate for the acetoclastic biomass if no substrate limitation or inhibition occurs. |
| H2-utilizing Mu Max | 1.4 | $d^{-1}$ | Maximum specific growth rate for the $H_2$-utilizing biomass if no substrate limitation or inhibition occurs. |
| Acetoclastic Ks | 100 | mgCOD/L | Half saturation for regulation of acetoclastic biomass growth rate, based on availability of acetate as substrate. |
| Acetoclastic | 0.5 | mgCOD/L | Half saturation concentration of |

| | | | |
|---|---|---|---|
| methanol Ks | | | methanol for acetoclastic biomass. |
| Hydrogenotrophic CO2 half sat. | 0.1 | mmol$CO_2$/L | Half saturation for regulation of $H_2$-utilizing biomass growth rate, based on availability of $CO_2$ as substrate. |
| H2-utilizing Ks | 0.1 | mgCOD/L | Half saturation for regulation of $H_2$-utilizing biomass growth rate, based on availability of hydrogen as substrate. |
| H2-utilizing methanol Ks | 0.5 | mgCOD/L | Half saturation concentration of methanol for $H_2$-utilizing biomass. |
| Acetoclastic propionic inhibition | 10000 | mgCOD/L | Propionate inhibition constant: high levels of propionate inhibit acetoclastic biomass growth. |
| Acetoclastic decay rate | 0.13 | $d^{-1}$ | Decay rate constant when there is no oxygen available. |
| Acetoclastic aerobic decay rate | 0.6 | $d^{-1}$ | Decay rate constant in the presence of oxygen. |
| H2-utilizing decay rate | 0.13 | $d^{-1}$ | Decay rate constant when there is no oxygen available. |
| H2-utilizing aerobic decay rate | 0.6 | $d^{-1}$ | Decay rate constant in the presence of oxygen. |

## *Stoichiometric*

Menu Location: **Project|Parameters|Stoichiometric|Methanogens**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Acetoclastic yield | 0.1 | mgCOD/mgCOD | Amount of acetoclastic biomass produced using one unit of substrate (acetate). The rest of the substrate will be converted to $CO_2$. |
| Methanol acetoclastic yield | 0.1 | mgCOD/mgCOD | Acetoclastic biomass yield on one unit of methanol COD. |
| H2-utilizing yield | 0.1 | mgCOD/mgCOD | Amount of $H_2$-utilizing biomass produced using one unit of substrate (hydrogen). The rest of the substrate will be converted to methane and water. |
| Methanol H2-utilizing yield | 0.1 | mgCOD/mgCOD | $H_2$-utilizing biomass yield on one unit of methanol COD |
| N in acetoclastic biomass | 0.07 | mgN/mgCOD | N content of acetoclastic biomass. |
| N in H2-utilizing biomass | 0.07 | mgN/mgCOD | N content of $H_2$-utilizing biomass. |
| N in acetoclastic endog. residue | 0.07 | mgN/mgCOD | N content of endogenous residue originating from acetoclastic decay. |

| | | | |
|---|---|---|---|
| H2-utilizing N in endog. Residue | 0.07 | mgN/mgCOD | N content of endogenous residue originating from $H_2$-utilizing biomass decay. |
| P in acetoclastic biomass | 0.022 | mgP/mgCOD | P content of acetoclastic biomass. |
| P in H2-utilizing biomass | 0.022 | mgP/mgCOD | P content of $H_2$-utilizing biomass. |
| P in acetoclastic endog. residue | 0.022 | mgP/mgCOD | P content of endogenous residue originating from acetoclastic decay. |
| P in H2-utilizing endog. Residue | 0.022 | mgP/mgCOD | P content of endogenous residue originating $H_2$-utilizing biomass. |
| Acetoclastic fraction to endog. residue | 0.08 | - | Fraction of acetoclastic biomass that becomes inert upon decay. |
| H2-utilizing fraction to endog. residue | 0.08 | - | Fraction of $H_2$-utilizing biomass that becomes inert upon decay. |
| Acetoclastic COD:VSS ratio | 1.42 | mgCOD/mgVSS | Conversion factor between biomass as measured in COD and its VSS content. This value is relatively stable for biomass. |
| H2-utilizing COD:VSS ratio | 1.42 | mgCOD/mgVSS | Conversion factor between biomass as measured in COD and its VSS content. This value is relatively stable for biomass. |

### *pH Inhibition*

Menu Location: **Project|Parameters|Kinetic|pH**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Acetoclastic methanogens low pH limit | 5 | pH units | At a pH equal to this value the growth rate of the methanogens will be reduced by 50%. Methanogens are sensitive to low pH, the digester can easily turn acid. |
| Acetoclastic methanogens high pH limit | 9 | pH units | At a pH equal to this value the growth rate of the methanogens will be reduced by 50% |
| H2-utilizing methanogens low pH limit | 5 | pH units | At a pH equal to this value the growth rate of the methanogens will be reduced by 50%. Methanogens are sensitive to low pH, the digester can easily turn acid. |
| H2-utilizing methanogens high pH limit | 9 | pH units | At a pH equal to this value the growth rate of the methanogens will be reduced by 50% |

### *Switching Functions*

Menu Location: **Project|Parameters|Kinetic|Switches**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Heterotrophic DO half sat. | 0.05 | $mgO_2/L$ | This constant is used to switch off aerobic OHO activity under low DO conditions (that is in anaerobic and anoxic reactors). |
| Anoxic NO3 half sat. | 0.1 | mgN/L | This constant is used to switch off anoxic growth processes using nitrate under low nitrate conditions. |
| Anoxic NO2 half sat. | 0.1 | mgN/L | This constant is used to switch off anoxic growth processes using nitrite under low nitrite conditions. |
| NH3 nutrient half sat. | 0.001 | mgN/L | This constant is used to slow all biomass growth processes at low ammonia-N concentrations (N nutrient limiting. |
| P nutrient half sat. | 0.001 | mgP/L | This constant is used to slow the growth of biomass when there is no phosphorus available as nutrient. |
| Synthesis anion/cation half sat. | 0.01 | meq/L | Half saturation concentration for anions and cations. |

# Chemical Precipitation Model

The Chemical Precipitation Model in BioWin describes insoluble metal salt formation that occurs in wastewater treatment plants under various environmental conditions. The objective of this model is to improve the prediction of soluble phosphate residuals and provide accurate chemical sludge production estimates. Phosphorus plays an active part both in biological and chemical processes in wastewater. It is an important part of the weak acid-base system, it is a nutrient and an energy-storage compound for various microorganisms and it readily forms insoluble precipitates with magnesium, calcium, as well as iron and aluminum ions if those are added to the wastewater. All these processes need to be taken into account for accurate effluent phosphorus predictions.

The Chemical Precipitation Model in BioWin contains the following functional categories, modules

**Chemical Phosphorus Precipitation by Alum or Ferric**

**Struvite and Calcium Phosphates Precipitation**

These modules are described in detail below.

## Ferric or Alum Precipitation

**Number of Reactions:** 6

**Engineering Objective:** Chemical phosphorus removal

**Implementation:** Optional, has to be activated in the BioWin model options

**Module Description:**

In the current implementation either Ferric or Aluminum phosphate precipitation can be selected as an option, but not both. Since precipitation is orders of magnitude faster than biological reactions, the model equations are expressed and solved using an equilibrium approach. The added metal will form an insoluble phosphate/hydroxo complex ($Fe_{1.6}H_2PO_4OH_{3.8}$ or $Al_{0.8}H_2PO_4OH_{1.4}$), a soluble metal-phosphate complex ($FeH_2PO_4^{2+}$ or $AlHPO_4^{+}$), and any residual metal will be mostly bound in metal hydroxide precipitate ($Fe(OH)_3$ or $Al(OH)_3$). In equilibrium there is always a low concentration of free metal ions and soluble phosphate species in various dissociated or undissociated forms ($PO_4^{3-}$, $HPO_4^{2-}$, $H_2PO_4^{-}$, $H_3PO_4$). The phosphate species together with the soluble metal-phosphate complex cause the residual, soluble effluent phosphorus concentration. The reactions are handled using the proper solubility and dissociation equations. The distribution and residual concentration of these components is pH and dose dependent. For soluble phosphorus species in case of a large metal overdose the following graphs show the pH sensitivity:

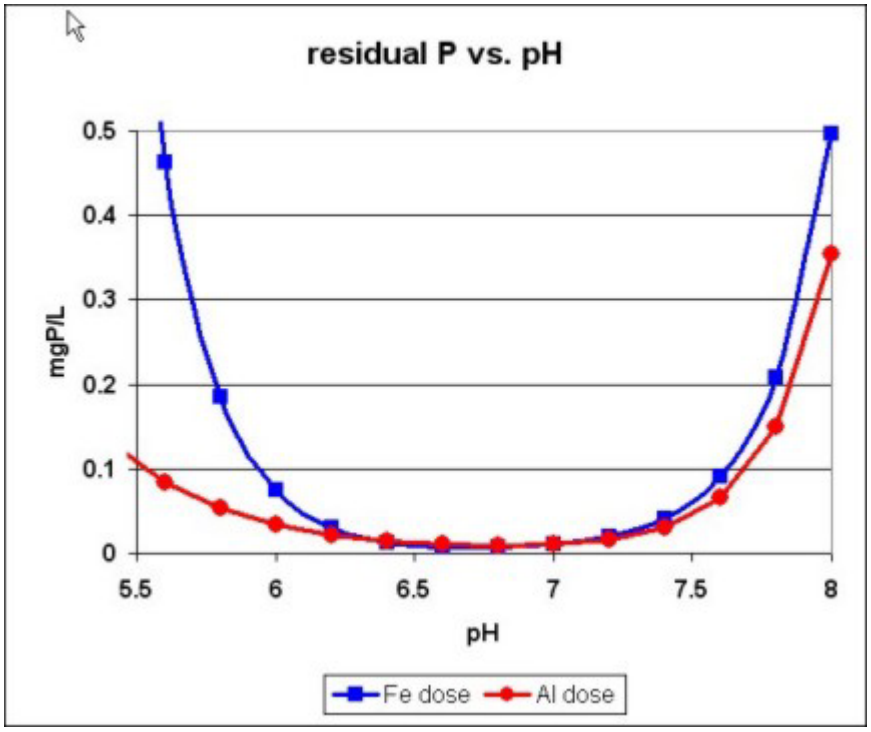



*Figure 1 : pH sensitivity for soluble phosphorus species in case of a large metal overdose*

Model parameters are listed in:

Menu Location: **Project|Parameters|Other|Physico-chemical constants**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|

| | | | |
|---|---|---|---|
| Equilibrium soluble PO4 with Al dosing at pH 7 | 0.01 | mgP/L | This is the best achievable soluble PO4 concentration when the solution is in equilibrium with the composite product of $Al_rH_2PO_4OH_{(3r-1)}$ based on the following reaction equation: $\left(Al^{3+}\right)^{0.8}\left(H_2PO_4^-\right)\left(OH^-\right)^{1.4} = K_{sp,AlP}$ $\left(Al^{3+}\right)^{0.8}\left(H_2PO_4^-\right)\left(OH^-\right)^{1.4} = K_{sp,AlP}$ |
| Al to P mole ratio (r) in $Alr(H_2PO_4)(OH)_3r-1$ precipitation | 0.8 | mmolAl/mmolP | Under low doses and optimal pH this is the default molar ratio between the precipitated aluminum and phosphate ions. However the actual (observed) ratio will depend on pH, as well as the formation of other aluminum phosphate and hydroxide components. |
| $Al(OH)_3$ solubility product | 1.2590E+9 | mol/L | This solubility constant is based on the reaction $Al^{3+} + 3H_2O \leftrightarrow Al(OH)_3 + 3H^+$, as expressed by: $\frac{\left(Al^{3+}\right)}{\left(H^+\right)^3} = K_{sp,AlOH3}$ The value of this constant should never be changed. The hydroxide precipitate formed in this reaction uses up aluminum ions and contributes to the non-stoichiometric Al/P ratios observed as well as the required overdose. |
| $AlHPO_4$+ dissociation constant | 7.9430E-13 | mol/L | This dissociation constant is based on the following reaction equation: $\frac{\left(Al^{3+}\right)\left(HPO_4^{2-}\right)}{\left(AlHPO_4^+\right)} = K_{iAlHPO4}$ This soluble aluminum phosphate complex will contribute to the residual soluble phosphate concentration measured. |
| Equilibrium soluble PO4 with Fe dosing at pH 7 | 0.01 | mgP/L | This is the best achievable soluble PO4 concentration when the solution is in equilibrium with the composite product of $Fe_{1.6}H_2PO_4OH_{3.8}$ based on the following reaction equation: $\left(Fe^{3+}\right)^r\left(H_2PO_4^-\right)\left(OH^-\right)^{3r-1} = K_{sp,FeP}$ |
| Fe to P mole ratio (r) in $Fer(H_2PO_4)(OH)_3r-1$ precipitation | 1.6 | mmolFe/mmolP | Under low doses and optimal pH this is the default molar ratio between the precipitated ferric and phosphate ions. However the actual (observed) ratio will depend on pH, as well as the formation of other ferric phosphate and hydroxide components. |
| $Fe(OH)_3$ solubility product | 0.05 | mol/L | This solubility constant is based on the reaction: $Fe^{3+} + 3H_2O \leftrightarrow Fe(OH)_3 + 3H^+$, as expressed by: |

| | | | |
|---|---|---|---|
| | | | $\frac{(Fe^{3+})}{(H^{+})^{3}} = K_{sp,FeOH3}$<br>The value of this constant should never be changed. The hydroxide precipitate formed in this reaction uses up ferric ions and contributes to the non-stoichiometric Fe/P ratios observed as well as the required overdose. |
| $FeH2PO_4$++ dissociation constant | 5.0120E-22 | mol/L | This dissociation constant is based on the following reaction equation:<br>$\frac{(Fe^{3+})(H_2PO_4^{-})}{(FeH_2PO_4^{2+})} = K_{iFeH_2PO_4}$<br>This soluble ferric phosphate complex will contribute to the residual soluble phosphate concentration measured. |

## Spontaneous Chemical Precipitation

**Module Description:**

Magnesium and Calcium is present in most wastewaters and can spontaneously form precipitates. From the large number of phosphate and carbonate precipitates that can be formed under typical conditions, particularly under higher than neutral pH, the most important ones affecting soluble phosphorus levels are struvite (magnesium-ammonium-phosphate, $MgNH_4PO_4 \cdot 6H_2O$), and hydroxy-dicalcium-phosphate (HDP, $Ca_2HPO_4(OH)_2$ ).

Struvite typically forms in digesters, due to the high concentration of magnesium, ammonium and phosphate ions present. These ions are transported to the digester in the biomass and are released. BioWin (in the anaerobic module) describes Mg, N, and P release. The resulting struvite precipitation can occur particularly in pipes and on overflow weirs, where degassing of $CO_2$ raises the pH. The model is described in detail in Musvoto et al. (2000).

HDP (and many other types of calcium phosphates) can precipitate in the bioreactor due to pH changes occurring in the anaerobic/aerobic zones. Accurate prediction of phosphate levels in bio-P processes may require simulating the HDP precipitation – redissolution phenomena as well. BioWin contains one more calcium phosphate precipitate, hydroxy-apatite (HAP), that is considered a sink for calcium that does not redissolve. The model is described in Maurer et al. (1999).

These precipitation processes are formulated with kinetic equations, according to the referenced papers.

**Number of Processes:** 3

**Engineering Objective:** Formation of Struvite and Calcium Phosphates

**Implementation:** Optional, has to be activated in the BioWin model options

Model parameters are listed in:

Menu Location: **Project|Parameters|Other|Physico-chemical rates**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|

| | | | |
|---|---|---|---|
| Struvite precipitation rate | 3.0000E+10 | $d^{-1}$ | The published precipitation rate (Musvoto et al. expressed in molar terms) is $3*10^{15}$. Simulation of other experiments suggests a much lower rate (Suzuki 1998). Mixing effects likely have an influence on the rate constant. The default selected is a compromise and can be changed in the range of $10^{9}$ to $3*10^{15}$. |
| Struvite redissolution rate | 3.0000E+11 | $d^{-1}$ | This constant has a lower importance as struvite redissolution is not typically encountered in wastewater processes. |
| Struvite half sat. | 1.0 | mgTSS/L | This is an empirical constant designed to provide continuity to the mathematical solution by maintaining low levels of struvite even under lower pH conditions. Its value should not be changed. |
| HDP precipitation rate | 1.0000E+8 | L/(molP.d) | The value of this rate constant will affect how close to equilibrium the HDP precipitation reaction will be under the given hydraulic resident times. If it is necessary to change it, it should be changed together with the redissolution rate constant. |
| HDP redissolution rate  | 1.0000E+8 | L/(molP.d) | The value of this rate constant will affect how close to equilibrium the HDP redissolution reaction will be under the given hydraulic residence times. If it is necessary to change it, it should be changed together with the precipitation rate constant. |
| HAP precipitation rate | 5.0000E-4 | molHDP/(L.d) | This constant rate will generate insoluble HAP that cannot be redissolved. |

Menu Location: **Project|Parameters|Other|Physico-chemical constants**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Struvite solubility product | 6.9180E-14 | mol/L | This solubility constant should not be changed |
| HDP solubility product | 2.7500E-22 | mol/L | This solubility constant should not be changed |
| HDP half sat. | 1.0 | mgTSS/L | This is an empirical constant designed to provide continuity to the mathematical solution by maintaining low levels of |

| | | | |
|---|---|---|---|
| | | | HDP even under lower pH conditions. Its value should not be changed. |

# Settling Models

**Engineering Objective:** Gravitational solid / liquid separation

**Implementation:** Flux-based solids / liquid separation models (used in one-dimensional model clarifier elements)

**Module Description:**

The general flux theory approach models solids settling in one dimension. In the one-dimensional approach solids and liquid movement in the vertical direction are assumed to be dominant and horizontal movement is ignored. The settling tank is divided into a number of layers in the vertical direction and a numerical technique is used to solve the mass balance equations in the vertical direction. The solution to the mass balance equations provides the solids concentration profile in the settling tank, and the solids concentration in the effluent and underflow. For more details, please see the **Flux Based Models** section of the "*Settling and Solid / Liquid Separation Models*" chapter.

BioWin offers two types of flux theory models:

**1 – Modified Vesilind**

**2 – Double Exponential**

Each model has its own set of parameters; these are described below.

## *Modified Vesilind Parameters*

Menu Location: **Project|Parameters|Settling|Modified Vesilind**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Maximum Vesilind settling velocity ($V_0$) | 170 | m/d | The maximum attainable settling velocity at theoretically infinite dilution in the unmodified Vesilind relationship. Primarily affects clarification function. Higher values are associated with well-settling sludge. |
| Vesilind hindered zone settling parameter (K) | 0.37 | L/g | The term which describes the exponential decrease in settling velocity with increasing concentration in the Vesilind relationship. Primarily affects the thickening function. Higher values associated with poor settling sludge. |
| Clarification switching function | 100 | mg/L | Switch applied in a Monod-type switching function to the Vesilind relationship. Addresses unrealistically high settling velocities predicted at low solids concentrations by strict application of the Vesilind model as originally published. Increasing the value for this switch will result in higher |

| | | | |
|---|---|---|---|
| | | | effluent suspended solids predictions. |
| Specified TSS conc.for height calc. | 2500 | mg/L | BioWin will locate and plot the height of the specified suspended solids concentration within the settler profile. |
| Maximum compactability constant | 15,000 | mg/L | The specified value is used to limit the maximum suspended solids concentration that can be achieved in a model settler layer. Also, as the solids concentration in a layer approaches this concentration, resuspension of solid particles occurs. |

## *Double Exponential Parameters*

Menu Location: **Project|Parameters|Settling|Double Exponential**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Maximum Vesilind settling velocity ($V_0$) | 410 | m/d | The maximum attainable settling velocity at theoretically infinite dilution in the unmodified Vesilind relationship. |
| Maximum (practical) settling velocity ($V_0'$) | 270 | m/d | The maximum settling velocity attainable in the Double Exponential model. This constraint addresses the unrealistically high settling velocities predicted at low solids concentrations by strict application of the Vesilind model. Higher values are associated with well-settling sludge. |
| Hindered zone settling parameter (Kh) | 0.40 | L/g | The term which describes the exponential decrease in settling velocity with increasing concentration in Zone 4 of the Double Exponential model where hindered settling dominates. Higher values associated with poor settling sludge. |
| Flocculent zone settling parameter (Kf) | 2.5 | L/g | The exponential term which describes settling behavior in Zone 2 of the Double Exponential model where flocculant settling is dominant. Higher values associated with poor settling sludge. |
| Maximum non-settleable TSS | 20 | mg/L | The minimum attainable suspended solids concentration in a layer is calculated as a fraction of the settling tank influent solids concentration, but it may not be less than this user-specified value. |
| Non-settleable fraction | 0.001 | - | The minimum attainable suspended solids concentration in a layer is calculated as a fraction of the settling tank influent solids concentration. |
| Specified TSS conc. for height calc. | 2500 | mg/L | BioWin will locate and plot the height of the specified suspended solids concentration within the settler profile. |

# pH Model

The **pH model** is described in detail in the *"Modeling of pH in BioWin"* chapter.

# Aeration and Gas Transfer Model

Parameters used in BioWin's aeration and gas transfer model are accessed via a number of different tabs. These are listed in the following sections.

**Number of Processes: 6**

**Engineering Objective:** Gas-liquid mass transfer

**Implementation:** permanent, always active in the BioWin model

**Module Description:**

There are six gas-liquid mass transfer processes to allow interphase transfer of oxygen, carbon-dioxide, methane, nitrogen, ammonia and hydrogen. Details about the mass transfer model may be found in the *"Gas-Liquid Mass Transfer"* chapter.

The Mass transfer model is impacted by the values of the following model parameters.

### *Mass transfer Parameters*

Menu Location: **Project|Parameters|Other|Mass transfer**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| $K_L$ for $H_2$ | 17.0 | m/d | Liquid phase mass transfer coefficient for $H_2$ |
| $K_L$ for $CO_2$ | 10.0 | m/d | Liquid phase mass transfer coefficient for $CO_2$ |
| $K_L$ for $NH_3$ | 1.0 | m/d | Liquid phase mass transfer coefficient for $NH_3$ |
| $K_L$ for $CH_4$ | 8.0 | m/d | Liquid phase mass transfer coefficient for $CH_4$ |
| $K_L$ for $N_2$ | 15.0 | m/d | Liquid phase mass transfer coefficient for $N_2$ |
| $K_L$ for $O_2$ | 13.0 | m/d | Liquid phase mass transfer coefficient for $O_2$ |

### *Aeration Parameters*

Menu Location: **Project|Parameters|Other|Aeration**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Alpha (surf) OR Alpha F (diff) | 0.50 | Unitless | $\alpha$ is the ratio of the overall mass transfer coefficient in process water to the overall mass transfer coefficient in clean water. F (diffuser fouling factor) is the ratio of the overall mass transfer coefficient for a particular diffuser after a given time in service to that of a new diffuser in the same process water. |

| | | | |
|---|---|---|---|
| Beta | 0.95 | Unitless | β is the ratio of the dissolved oxygen saturation concentration in process water to the saturation concentration in clean water |
| Surface pressure | 101.325 | kPa | Atmospheric pressure at field conditions. |
| Fractional effective saturation depth (Fed) | 0.325 | Unitless | The effective saturation depth is the depth at which the total pressure (hydrostatic and atmospheric) would produce a saturation concentration equal to the steady state saturation concentration for the system. |
| Supply gas CO2 | 0.035 | vol. % | The volume percentage of carbon dioxide in the supply gas to a diffused air system. This parameter is also used to determine the dissolved carbon dioxide saturation concentration for surface aerator systems. |
| Supply gas O2 | 20.95 | vol. % | The volume percentage of oxygen in the supply gas to a diffused air system. This parameter is also used to determine the dissolved oxygen saturation concentration for surface aerator systems. |
| Off-gas CO2 | 2.0 | vol. % | The volume percentage of carbon dioxide in the gas leaving a diffused air system. [This parameter is not used if the gas phase is modeled.] |
| Off-gas O2 | 18.8 | vol. % | The volume percentage of oxygen in the gas leaving a diffused air system. [This parameter is not used if the gas phase is modeled.] |
| Off-gas H2 | 0.00 | vol. % | The volume percentage of hydrogen in the gas leaving a diffused air system. [This parameter is not used if the gas phase is modeled.] |
| Off-gas NH3 | 0.00 | vol. % | The volume percentage of ammonia in the gas leaving a diffused air system. [This parameter is not used if the gas phase is modeled.] |
| Surface turbulence factor | 2 | Unitless | This parameter indicated the intensity of mixing on the surface conditions (it has little impact in aerated systems). |
| Set point controller gain | 1.0 | Unitless | This parameter may be used to increase the gain of the dissolved oxygen controller. Typically the user would increase this value if the controller was slow in achieving the dissolved oxygen set point. |

## *Diffuser Parameters*

Location: '**Model Parameters' on Element "Operation" tab**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| $k_1$ in $C = k_1(PC)^{0.25}$ | 2.5656 | | Correlation parameter |

| | | | |
|---|---|---|---|
| $+ k_2$ | | | |
| $k_2$ in $C = k_1(PC)^{0.25} + k_2$ | 0.04320 | | Correlation parameter |
| Y in $K_La = C\ Usg^Y$ | 0.82000 | | Correlation parameter |
| Area of one diffuser | 0.04100 | $m^2$ | Area of a single diffuser is required to determine the number of diffusers. |
| % of tank area covered by diffusers (PC) | 10.00000 | % | Ratio of the total active diffuser area to the tank area as a percentage. |
| Diffuser mounting height | 0.25 | m | Height of diffuser discharge above tank floor |
| Min. air flow rate per diffuser | 0.50000 | $m^3\ hr^{-1}$ | Minimum of X axis in SOTE plot. |
| Max. air flow rate per diffuser | 10.00 | $m^3\ hr^{-1}$ | Maximum of X axis in SOTE plot. |

### *Surface aerator Parameters*

Location: '**Model Parameters' on Element "Operation" tab**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|
| Surface aerator Std. oxygen transfer rate | 1.500000 | kg O $kW^{-1}\ hr^{-1}$ | Standard oxygen transfer rate for rotary surface aerators |
| Maximum power per rotor | 20.00000 | kW | The maximum power input per surface aerator is used to determine the number of aerators required. |

# Model Library for the Model Builder

The following builder models have been included with BioWin:

- ASM1
- ASM2d
- ASM3
- Aerobic growth of methylotrophs on methanol
- Inert conversion
- $CaCO_3$ precipitation

For more information on loading these models, and using the Model Builder interface in general, please see the **Model Builder** section of the *"Useful BioWin Interface Tools and Techniques"*chapter.

The following points should be noted when using these Builder models:

- **OURc** – the displayed value for this parameter is the carbonaceous OUR for the BioWin model only. Therefore when a Model Builder model is active, oxygen demand from any user-defined processes are not included (OURn is similar but only applies to the oxygen utilized for AOB and NOB growth). In summary, OURc and OURn only reflect the BioWin model terms; if there is no BioWin model used in the Model Builder then they will be zero.
- **OURt** is calculated from the sum of all process rates that use or produce oxygen. Consequently if the BioWin reactions are ON in the model builder then:
- **OURt - OURn - OURc** = the **OUR** from the Model Builder reactions
- and if BioWin reactions are **Off** in the **Model Builder** then:
- **OURt** = the **OUR** from the Model Builder reactions.

# Definition of Combined Variables

To model the range of system types it is necessary to track the concentrations of a large number of components (state variables) in each stream of a configuration. In certain cases tracking a number of the variables may be superfluous. For example, if a system incorporates only an aerobic activated sludge unit then all variables relating to biological phosphorus removal will have zero concentration values (polyP heterotrophic organism mass, stored polyphosphate, etc.).

Each element in the configuration is modeled to provide a mass balance on the following state variables.

| Short name | Full name | Units |
|---|---|---|
| Zbh | Non-polyP heterotrophs | [mgCOD/L] |
| Zbmeth | Anoxic methanol utilizers | [mgCOD/L] |
| Zaob | Ammonia oxidizing biomass | [mgCOD/L] |
| Znob | Nitrite oxidizing biomass | [mgCOD/L] |
| Zamox | Anaerobic ammonia oxidizers | [mgCOD/L] |
| Zbp | PolyP heterotrophs | [mgCOD/L] |
| Zbpa | Propionic acetogens | [mgCOD/L] |
| Zbam | Acetoclastic methanogens | [mgCOD/L] |
| Zbhm | Hydrogenotrophic methanogens | [mgCOD/L] |
| Ze | Endogenous products | [mgCOD/L] |
| Xsp | Slowly bio. COD (part.) | [mgCOD/L] |
| Xsc | Slowly bio. COD (colloid.) | [mgCOD/L] |
| Xi | Part. inert. COD | [mgCOD/L] |
| Xon | Part. bio. org. N | [mgN/L] |
| Xop | Part. bio. org. P | [mgP/L] |
| Xin | Part. inert N | [mgN/L] |

| | | |
|---|---|---|
| Xip | Part. inert P | [mgP/L] |
| Spha | Stored PHA | [mgCOD/L] |
| PP-lo | Releasable stored polyP | [mgP/L] |
| PP-hi | Fixed stored polyP | [mgP/L] |
| XPPCat | PolyP bound cations | [mg/L] |
| Sbsc | Readily bio. COD (complex) | [mgCOD/L] |
| Sbsa | Acetate | [mgCOD/L] |
| Sbsp | Propionate | [mgCOD/L] |
| Sbmeth | Methanol | [mgCOD/L] |
| SbH2 | Dissolved H2 | [mgCOD/L] |
| CH4 | Dissolved methane | [mg/L] |
| NH3-N | Ammonia N | [mgN/L] |
| Nos | Sol. bio. org. N | [mgN/L] |
| NO2-N | Nitrite N | [mgN/L] |
| NO3-N | Nitrate N | [mgN/L] |
| N2 | Dissolved nitrogen gas | [mgN/L] |
| PO4-P (incl. MeP) | PO4-P (Sol. & Me Complexed) | [mgP/L] |
| Sus | Sol. inert COD | [mgCOD/L] |
| Nus | Sol. inert TKN | [mgN/L] |
| ISS | Inorganic S.S. | [mgTSS/L] |
| XStru | Struvite | [mgTSS/L] |
| XHDP | Hydroxy-dicalcium-phosphate | [mgTSS/L] |
| XHAP | Hydroxy-apatite | [mgTSS/L] |
| SMg | Magnesium | [mg/L] |
| SCa | Calcium | [mg/L] |
| Me | Metal | [mg/L] |
| SCat | Other Cations (strong bases) | [meq/L] |
| SAn | Other Anions (strong acids) | [meq/L] |
| SCO2 | Total CO2 [mmol/L] | [mmol/L] |
| UD1 | User defined 1 | [mg/L] |
| UD2 | User defined 2 | [mg/L] |
| UD3 | User defined 3 [mgVSS/L] | [mgVSS/L] |
| UD4 | User defined 4 | [mgTSS/L] |
| DO | Dissolved oxygen | [mg/L] |
| Flow | Flow | Unit system dependant |
| Liq.Vol. | Liquid volume | Unit system dependant |
| Temp. | Temperature | Degrees celcius |

BioWin calculates a number of combined variables that may be displayed for certain elements. The following table outlines these combined variables.

| Short name | Full name | Description |
|---|---|---|

| | | |
|---|---|---|
| VSS | Volatile suspended solids | VSS is calculated converting all particulate COD state variables (biomasses, substrates and inert organics) with their proper COD/VSS ratios to VSS, adding User Defined Variable #3 and summing them. Biomasses have their own Fcv (COD/VSS) conversion factors, while for other components the ratios indicated in the **Project\|Parameters\|Other\|General** dialog are used. The VSS is calculated as follows:<br>VASS + Ze/Fcv,$_{ZBH}$ + Xsp/Fcv,$_{XSP}$ + Xi/Fcv,$_{XI}$ + Sphb/Fcv,$_{XSP}$ +UD3 |
| VASS | Volatile active suspended solids | VASS is calculated converting all biomass state variables with their proper COD/VSS ratios to VSS, and summing them. Biomasses have their own Fcv (COD/VSS) conversion factor in the proper stoichiometric parameter forms. The VASS is calculated as follows:<br>Zbh/Fcv,$_{ZBH}$+ Zbmeth/Fcv,$_{ZBMETH}$ + Zbaob/Fcv,$_{ZBAOB}$ + Zbnob/Fcv,$_{ZBNOB}$ + Zbanammox/Fcv,$_{ZBANAMMOX}$ + Zbp/Fcv,$_{ZBP}$ + Zbpa/Fcv,$_{ZBPA}$ + Zbam/Fcv,$_{ZBAM}$ + Zbhm/Fcv,$_{ZBHM}$ |
| TISS | Total inorganic suspended solids | TISS is the sum of inorganic solids from the influent (ISS), total precipitated solids, the poly-P content, UD4, and the organism ash content; that is:<br>XPrec + ISS + PP-lo + PP-hi +XPPCat + UD4 + (VASS + Ze/Fcv,$_{ZBH}$)*(1/(1-AshContent/100.0) - 1.0) |
| TSS | Total suspended solids | TSS is calculated as a sum of VSS and TISS. |
| XCOD | Particulate COD | Particulate COD is calculated as the sum of all particulate state variables that are expressed in COD, as follows:<br>Zbh + Zbmeth + Zba + Zbp + Zbpa + Zbam + Zbhm + Ze + Xsp + Xi +Sphb |
| SCOD | Filtered COD | Filtered COD is calculated as the sum of all soluble state variables that are expressed in COD, including the colloids and hydrogen as follows:<br>Sbsc + Sbsa + Sbsp + SbMeth + Sh2 + Sus + Xsc |
| COD | Total Chemical Oxygen Demand | Total COD is the sum of filtered and particulate COD. |
| $SPO_4$ | Soluble $PO_4$-P | Soluble $PO_4$-P is the sum of all inorganic phosphate species, including soluble metal phosphate complexes in case of metal dosage. Note that biodegradable and unbiodegradable soluble and colloidal organic P is considered zero. That is:<br>(SolubleP & Metal-complexed P) - ($Me_rH_2PO_4OH_{3r-1}$) |
| TP | Total P | Total P is calculated as the sum of Soluble $PO_4$-P, P content of biomasses and endogenous residue as a fraction, particulate inert and biodegradable organic P, P in releasable and fixed polyphosphate, and P bound in Struvite, HDP, HAP and metal phosphate precipitate if applicable. That is:<br>Zbh*Fzbp,$_{ZBH}$ + Zbmeth*Fzbp,$_{ZBMETH}$ + Zbaob*Fzbp,$_{ZBAOB}$+ Zbnob*Fzbp,$_{ZBNOB}$+ Zbanammox*Fzbp,$_{ZBANAMMOX}$ + Zbp*Fzbp,$_{ZBP}$ + Zbpa*Fzbp,$_{ZBPA}$ + Zbam*Fzbp,$_{ZBAM}$ + Zbhm* Fzbp,$_{ZBHM}$ + PP-lo + PP-hi + Xip + (SolubleP & |

| | | |
|---|---|---|
| | | Metal-complexed P) + Xop + Xstru *(MWPhosphorus/MWStru) + XHDP*(MWPhosphorus/MWXHDP) + XHAP*(3*MWPhosphorus)/MWXHAP |
| XPrec | Total precipitated solids | Precipitated solids are calculated as the sum of HDP, HAP, Struvite, Metal phosphate and metal hydroxide solids, that is:<br>XHDP + XHAP + Xstru + $MeOH_3$+ $Me_rH_2PO_4OH_{3r-1}$ |
| STKN | Filtered TKN | Filtered TKN is ammonia-N, and soluble biodegradable and unbiodegradable organic nitrogen, that is:<br>NH3 + Nos + Nus |
| XTKN | Particulate TKN | Particulate TKN is calculated as the sum of the N content of biomasses, particulate inert and biodegradable organic N, and the N content of struvite; that is:<br>$Zbh*Fzbn_{,ZBH}$ + $Zbmeth*Fzbn_{,ZBMETH}$ + $Zbaob*Fzbn_{,ZBAOB}$ + $Zbnob*Fzbn_{,ZBNOB}$ + $Zbanammox*Fzbn_{,ZBANAMMOX}$ + $Zbp*Fzbn_{,ZBP}$ + $Zbpa*Fzbn_{,ZBPA}$ + $Zbam*Fzbn_{,ZBAM}$ + $Zbhm*Fzbn_{,ZBHM}$ + $X_{IN}$ + $X_{ON}$ + XStru * MWNitrogen/MWStru |
| TKN | Total Kjeldahl Nitrogen | Total TKN is the sum of filtered and particulate TKN |
| TSBOD | Filtered Carbonaceous BOD | See BOD section below |
| TCBOD | Total Carbonaceous BOD | See BOD section below |
| RBCOD | Readily biodegradable COD | RBCOD is the sum the VFA-COD, the complex readily biodegradable substrate and methanol, that is:<br>Sbsc + Sbsa + Sbsp + SbMeth |
| VFA | Volatile fatty acids | VFAs are calculated as the sum of acetate and propionate, that is:<br>Sbsa + Sbsp |
| TN | Total N | TN is TKN and nitrate-N, that is:<br>TKN+$NO_3$-N |
| TIN | Total inorganic N | TIN is ammonium, nitrate and struvite N, that is:<br>$NO_3$ + $NH_3$ + (Xstru * MWNitrogen/MWStru) |
| Alk | Alkalinity | Alkalinity is calculated from weak acid/base chemistry – see the "*Modeling of pH in BioWin*" chapter. |
| pH | pH | pH is calculated from weak acid/base chemistry – see the "*Modeling of pH in BioWin*" chapter. |

**Project|Parameters|Other|General**

| Name | Default Value | Unit | Explanation |
|---|---|---|---|

| | | | |
|---|---|---|---|
| Particulate substrate COD:VSS ratio | 1.60 | mgCOD/mgVSS | Conversion factor between particulate substrate as measured in COD and its VSS content. The average of this value and the biomass COD:VSS ratio will lead to the typical 1.48 mgCOD/mgVSS ratio found in activated sludge. |
| Particulate inert COD:VSS ratio | 1.60 | mgCOD/mgVSS | Conversion factor between particulate inert as measured in COD and its VSS content. |
| Ash content of biomass (synthesis ISS) | 8.00 | % | Ash content of biomass. ISS generated (uptake of minerals and micronutrients) by biomass growth. |
| Molecular weight of other anions | 35.50 | mg/mmol | Assume molecular weight of "other anions" state variable. |
| Molecular weight of other cations | 39.10 | mg/mmol | Assume molecular weight of "other cations" state variable. |
| Mg to P mole ratio in polyphosphate | 0.30 | mmol Mg/mmol P | Mole ratio of magnesium to phosphorus in polyphosphate. |
| Cation to P mole ratio in polyphosphate | 0.30 | meq/mmol P | Mole ratio of magnesium to phosphorus in polyphosphate. |
| Ca to P mole ratio in polyphosphate | 0.05 | mmol Ca/mmol P | Mole ratio of calcium to phosphorus in polyphosphate. |
| Bubble rise velocity (anaerobic digester) | 23.9 | cm/s | The bubble rise velocity is used to calculate the gas holdup in anaerobic digesters. Increasing the rise velocity will decrease the gas holdup. |
| Bubble Sauter mean diameter (anaerobic digester) | 0.35 | cm | The Sauter mean diameter is the diameter of a sphere with the same volume to surface ratio as the volume to surface ratio of the total dispersion. |
| Anaerobic digester gas hold-up factor | 1 | | This parameter can be used to adjust the digester mass transfer. |
| Tank head loss per metre of length (from flow) | 0.0025 | m/m | This parameter is used to calculate the power dissipation from flow. |
| Minimum air flow (per unit volume) without mixing | 1 | $m^3/(m^3 d)$ | |

# COD and BOD in BioWin

In the BioWin simulator characterization of the carbonaceous material in municipal wastewater is in terms of the chemical oxygen demand (COD). This selection is based on a number of factors, but primarily because COD provides a consistent basis for description of the activated sludge process, and for quantifying sludge production, oxygen demand, etc. The rationale for preferring COD over other

parameters such as biochemical oxygen demand (BOD) or total organic carbon (TOC) is discussed in this section.

The simulator allows for calculation of soluble and total BOD for any input element, process unit, or stream. The user may specify the time basis for the BOD calculation (5, 7, or 20 days).

In many instances data on treatment plant operation are recorded in terms of the BOD for both the influent and effluent, usually reported as the 5-day value ($BOD_5$). This section discusses a number of factors regarding the application of BioWin where data are recorded on a BOD basis, or where there is a requirement to quantify effluent BOD levels for regulatory purposes.

## BOD Calculations in BioWin

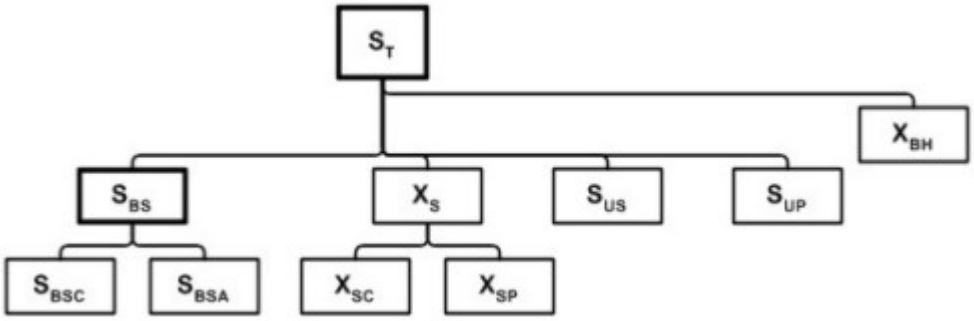
The basis for modeling organic components in BioWin is the chemical oxygen demand (COD) parameter. However, BioWin allows for calculation of soluble (filtered) and total carbonaceous biochemical oxygen demand (BOD) for any input element, process unit, or stream. The user may specify the time basis for the BOD calculation (5, 7, or 20 days).

Calculation of BOD is based on differing rates of degradation of the different components (*e.g.,* influent biodegradable material (readily and slowly biodegradable), active organism masses which exert an endogenous oxygen demand and hence a BOD, *etc*.). Essentially BioWin uses analytical equations to estimate BOD.

The objective here is to demonstrate the method used by BioWin in calculating filtered and total BOD concentrations, and show how the equations were developed. Understanding development of the equations presented below is facilitated by the figure below which illustrates the division of a wastewater stream into the different components.

| **Definition of Terms** | |
|---|---|
| B | Endogenous decay rate constant ($\cong 0.24\ d^{-1}$) |
| $BOD_E$ | Biochemical oxygen demand due to endogenous respiration |
| $BOD_S$ | Soluble component of biochemical oxygen demand |
| $BOD_{XSP}$ | Particulate slowly biodegradable component of biochemical oxygen demand |
| $BOD_{XBH}$ | Active biomass component of biochemical oxygen demand |
| $BOD_T$ | Total biochemical oxygen demand |
| $f$ | Fraction of active mass remaining as endogenous residue ($\cong 0.20$) |
| $f_{BS}$ | Fraction of total influent COD which is readily biodegradable |
| $f_{UP}$ | Fraction of total influent COD which is unbiodegradable particulate |
| $f_{US}$ | Fraction of total influent COD which is unbiodegradable soluble |
| $f_{XBH}$ | Fraction of total influent COD which is active organisms |
| $f_{XSP}$ | Fraction of slowly degradable COD which is particulate |
| K | First order rate constant for $X_{SP}$ degradation ($\cong 0.40\ d^{-1}$) |
| $(MO_2)_G$ | Mass of oxygen utilized for growth on soluble substrate |
| $(MO_2)_E$ | Mass of oxygen utilized for endogenous metabolism |
| OUR | Oxygen utilization rate (mg/L/day) |

| | |
|---|---|
| $OUR_E$ | Oxygen utilization rate due to endogenous metabolism |
| $OUR_G$ | Oxygen utilization rate for substrate utilization (growth) |
| $S_{BS}$ | Soluble readily biodegradable COD concentration (mg COD/L) |
| $S_{BSA}$ | Soluble readily biodegradable volatile fatty acid COD concentration (mg COD/L) |
| $S_{BSP}$ | Soluble readily biodegradable propionate COD concentration (mg COD/L) |
| $S_{BMETH}$ | Soluble readily biodegradable methanol COD concentration (mg COD/L) |
| $S_{BSC}$ | Soluble readily biodegradable complex COD concentration (mg COD/L) |
| $S_S$ | Soluble (filtered) biodegradable COD concentration (mg COD/L) |
| $S_{UP}$ | Particulate unbiodegradable COD concentration (mg COD/L) |
| $S_{US}$ | Soluble unbiodegradable COD concentration (mg COD/L) |
| $S_T$ | Total COD concentration (mg COD/L) |
| T | Time (d) |
| $X_{BH}$ | Active organism concentration (*i.e.* the sum of seven organism concentrations) (mg COD/L) |
| $X_{BH0}$ | Active organism concentration at time zero (mg COD/L) |
| $X_S$ | Slowly biodegradable COD concentration (mg COD/L) |
| $X_{SC}$ | Slowly biodegradable colloidal COD concentration (mg COD/L) |
| $X_{SP}$ | Slowly biodegradable particulate COD concentration (mg COD/L) |
| $X_{SP0}$ | Slowly biodegradable particulate COD concentration at time zero (mg COD/L) |
| Y | Yield of active organisms (≅ 0.666 mg cell COD mg $COD^{-1}$) |




*Division of municipal wastewater COD into constituent fractions*

## Basis for BOD Calculations

The approach for calculating BOD is to distinguish three components, and to calculate the BOD contribution for each component independently. These components are as follows:

1. BOD associated with utilization of soluble COD (both readily biodegradable and colloidal slowly biodegradable) and the biomass generated from this utilization;

2. BOD associated with utilization of slowly biodegradable particulate COD and the biomass generated from this utilization; and
3. BOD exerted by active biomass present in the sample. That is, biomass initially present; not biomass generated through utilization referred to in 1 and 2.

The simulator provides values for $S_{BSC}$, $S_{BSA}$, $X_{SC}$, $X_{SP}$ and $X_{BH}$ in any stream or process unit. When calculating BOD concentrations for input streams, the influent fractions provided by the user (or the default values) are used to calculate the appropriate concentrations.

## BOD Associated with Soluble Biodegradable COD ($S_S$):

For the purpose of BOD calculations, the "soluble" biodegradable COD ($S_S$) can be considered to be the sum of the readily biodegradable COD ($S_{BSC} + S_{BSA} + S_{BSP} + S_{BMETH}$) and the biodegradable colloidal COD ($X_{SC}$), *i.e.,*

$$S_S = S_{BSC} + S_{BSA} + S_{BSP} + S_{BMETH} + X_{SC} \quad (1)$$

$$S_S = S_{BSC} + S_{BSA} + S_{BSP} + S_{BMETH} + X_{SC} \quad (1)$$

The oxidation of this material occurs rapidly, and for the purpose of these calculations is assumed to occur instantaneously (*i.e.,* at t = 0). Assuming that the soluble biodegradable COD is oxidized instantly to form new cells:

$$S_S \rightarrow X_{BH0} = Y \cdot S_S \quad (\text{at time } t = 0) \quad (2)$$

then the mass of oxygen consumed for growth of these organisms $(MO_2)_G$ is:

$$(MO)_G = (1 - Y) \cdot S_S \quad (3)$$

Assuming that the rate of change in organism concentration due to endogenous decay is first order with respect to the active organism concentration, an expression for active organism concentration can be obtained, *i.e.*,

$$\frac{dX_{BH}}{dt} = -b \cdot X_{BH} \quad (4)$$

Therefore,

$$X_{BH} = X_{BH0} \cdot e^{-b\,t} \quad (5)$$

The BOD due to endogenous metabolism by the organisms generated from growth on $S_S$ can then be calculated using either of the methods described below.

**Method 1:**

From Eq.2 and Eq.5 , the endogenous mass loss at time t can be calculated:

$$\begin{aligned} \Delta X_{BH} &= X_{BH0} - X_{BH} \\ &= X_{BH0} \cdot (1 - e^{-b\,t}) \\ &= Y \cdot S_S \cdot (1 - e^{-b\,t}) \end{aligned} \quad (6)$$

and the mass of oxygen consumed for endogenous metabolism:

$$
\begin{aligned}
(MO)_E &= (1-f)\cdot \Delta X_{BH} \\
&= (1-f)\cdot Y \cdot S_S \cdot (1-e^{-b\,t})
\end{aligned}
\tag{7}
$$

This is equal to the BOD due to endogenous decay, *i.e.,*

$$
\begin{aligned}
BOD_E &= (1-f)\cdot X_{BH0}\cdot (1-e^{-b\,t}) \\
&= (1-f)\cdot Y \cdot S_S \cdot (1-e^{-b\,t})
\end{aligned}
\tag{8}
$$

The soluble BOD component can now be calculated by summing Eq. 3 and Eq. 8, *i.e.,*

$$
\begin{aligned}
BOD_S &= (MO)_G + (MO)_E \\
&= (1-Y)\cdot S_S + (1-f)\cdot Y \cdot S_S \cdot (1-e^{-b\,t})
\end{aligned}
\tag{9}
$$

**Method 2:**

The OUR due to endogenous metabolism can also be related to the rate of change in active organism concentration (taking into account that a fraction of the active mass becomes endogenous residue), *i.e.,*

$$
\begin{aligned}
OUR_E &= -(1-f)\cdot \frac{dX_{BH}}{dt} \\
&= b\cdot (1-f)\cdot X_{BH} \\
&= b\cdot (1-f)\cdot X_{BH0}\cdot e^{-b\,t}
\end{aligned}
\tag{10}
$$

The BOD due to endogenous decay is then the cumulative mass of oxygen used over time, *i.e.,*

$$
\begin{aligned}
BOD_E &= \int_0^t OUR_E\, dt \\
&= b\cdot (1-f)\cdot X_{BH0}\int_0^t e^{-b\,t} dt \\
&= b\cdot (1-f)\cdot X_{BH0}\cdot \left(-\frac{1}{b}e^{-b\,t}\right) + C \\
&= -(1-f)\cdot X_{BH0}\cdot e^{-b\,t} + C
\end{aligned}
\tag{11}
$$

and since at t = 0, $BOD_E = 0$,

$$C = (1+f)\cdot X_{BH0}$$

Substituting the expression obtained for $X_{BHO}$ (Eq. 2) into the above gives an expression for the BOD due to endogenous decay:

$$
\begin{aligned}
BOD_E &= -(1-f)\cdot X_{BH0}\cdot e^{-b\,t} + (1-f)\cdot X_{BH0} \\
&= (1-f)\cdot X_{BH0}\cdot (1-e^{-b\,t}) \\
&= (1-f)\cdot Y \cdot S_S \cdot (1-e^{-b\,t})
\end{aligned}
\tag{12}
$$

This is the same expression obtained using Method 1 (Eq. 8). The total soluble BOD portion is given by Eq. 9.

## BOD Associated with Slowly Biodegradable Particulate COD ($X_{SP}$):

The biochemical oxygen demand related to the slowly biodegradable particulate material can be calculated from the cumulative oxygen consumption for growth on $X_{SP}$ and endogenous respiration exerted by organisms from this growth. The OUR is the sum of two components:

$$\begin{aligned} OUR &= OUR_G + OUR_E \\ &= (1 - Y) \cdot \left( - \frac{dX_{SP}}{dt} \right) + (1 - f) \cdot \left( - \frac{dX_{BH}}{dt} \right)_E \\ &= (1 - Y) \cdot \left( - \frac{dX_{SP}}{dt} \right) + (1 - f) \cdot \left( bX_{BH} \right) \end{aligned} \tag{13}$$

The rate of change in slowly biodegradable particulate substrate concentration is assumed to be first order with respect to substrate concentration, *i.e.*,

$$\frac{dX_{SP}}{dt} = -k \cdot X_{SP}$$

Therefore,

$$X_{SP} = X_{SP0} \cdot e^{-kt} \tag{14}$$

The active organism concentration in Eq. 11 is obtained by integrating an expression for the rate of change of $X_{BH}$. This rate is a consequence of an increase due to growth on $X_{SP}$, minus a decrease due to endogenous metabolism, *i.e.*,

$$\frac{dX_{BH}}{dt} = Y \cdot \left( - \frac{dX_{SP}}{dt} \right) - b \cdot X_{BH} \tag{15}$$

Substituting Eq. 14 into the above results in a linear differential equation for $X_{BH}$ as a function of time, *i.e.,*

$$\begin{aligned} \frac{dX_{BH}}{dt} &= - Y \cdot \frac{dX_{SP}}{dt} - b \cdot X_{BH} \\ &= -Y \frac{d}{dt} \left( X_{SP0} \cdot e^{-kt} \right) - b \cdot X_{BH} \\ &= kYX_{SP0} \cdot e^{-kt} - b \cdot X_{BH} \end{aligned} \tag{16}$$

Or equivalently,

$$\frac{dX_{BH}}{dt} + b \cdot X_{BH} = kYX_{SP0} \cdot e^{-kt} \tag{17}$$

An integration factor of $e^{bt}$ can be used to solve the differential equation. Multiplying both sides of the equation by $e^{bt}$ results in a simplified expression:

$$\begin{aligned} e^{bt} \cdot \frac{dX_{BH}}{dt} + b \cdot e^{bt} \cdot X_{BH} &= e^{bt} \cdot kYX_{SP0} \cdot e^{-kt} \\ \frac{d}{dt} (e^{bt} \cdot X_{BH}) &= kYX_{SP0} \cdot e^{(b-k)t} \end{aligned} \tag{18}$$

Integrating both sides of Eq. 18:

$$(e^{bt} \cdot X_{BH}) = \int kYX_{SP0} \cdot e^{(b-k)t}\, dt$$

$$(e^{bt} \cdot X_{BH}) = \frac{kYX_{SP0}}{(b-k)} \cdot e^{(b-k)t} + C \qquad (19)$$

$$X_{BH} = \left(\frac{kYX_{SP0}}{b-k}\right) \cdot e^{-kt} + Ce^{-bt}$$

At t = 0 $X_{BH} = X_{BHO}$, therefore solving for **C** gives:

$$X_{BH} = \left(\frac{kYX_{SP0}}{b-k}\right) \cdot e^{-kt} + \left(X_{BH0} - \frac{kYX_{SP0}}{b-k}\right) \cdot e^{-bt} \qquad (20)$$

Returning to Eq. 13 for the oxygen utilization rate and substituting for $X_{BH}$:

$$\begin{aligned} OUR &= (1-Y) \cdot \left(-\frac{dX_{SP}}{dt}\right) + (1-f) \cdot (bX_{BH}) \\ &= (1-Y) \cdot kX_{SP} + (1-f) \cdot bX_{BH} \\ &= (1-Y) \cdot kX_{SP0} \cdot e^{-kt} + (1-f) \cdot b \cdot \left[\left(\frac{kYX_{SP0}}{b-k}\right) \cdot e^{-kt} + \left(X_{BH0} - \frac{kYX_{SP0}}{b-k}\right) \cdot e^{-bt}\right] \end{aligned} \qquad (21)$$

Integrating Eq. 21 gives an expression for the BOD of the slowly biodegradable material as a function of time, *i.e.,*

$$\begin{aligned} BOD_{XSP} &= \int_0^t OUR\, dt \\ &= \int_0^t (1-Y) \cdot kX_{SP0} \cdot e^{-kt} + (1-f) \cdot b \cdot \left[\left(\frac{kYX_{SP0}}{b-k}\right) \cdot e^{-kt} + \left(X_{BH0} - \frac{kYX_{SP0}}{b-k}\right) \cdot e^{-bt}\right] dt \\ &= -(1-Y) \cdot X_{SP0} \cdot e^{-kt} - \frac{(1-f) \cdot bYX_{SP0}}{(b-k)} \cdot e^{-kt} - (1-f) \cdot \left(X_{BH0} - \frac{kYX_{SP0}}{b-k}\right) \cdot e^{-bt} \\ &\quad + (1-Y) \cdot X_{SP0} + \frac{(1-f) \cdot bYX_{SP0}}{(b-k)} + (1-f) \cdot \left(X_{BH0} - \frac{kYX_{SP0}}{b-k}\right) \end{aligned}$$

Assuming $X_{BHO} \approx 0$ and re-arranging the above expression,

$$BOD_{XSP} = X_{SP0} \cdot \left[\left((1-Y) + \frac{(1-f) \cdot bY}{(b-k)}\right) \cdot \left(1 - e^{-kt}\right) - \left(\frac{(1-f) \cdot Yk}{(b-k)}\right) \cdot \right. \qquad (22)$$

The total BOD (if no biomass is present) is then the sum of $BOD_S$ and $BOD_{XSP}$,. (Eqs. 9 and 22), *i.e.,*

$$BOD_T = X_{SP0} \cdot \left[\left((1-Y) + \frac{(1-f) \cdot bY}{(b-k)}\right) \cdot \left(1 - e^{-kt}\right) - \left(\frac{(1-f) \cdot Yk}{(b-k)}\right) \cdot \left(1 - e^{-bt}\right)\right] \qquad (23)$$

$$+ (1-Y) \cdot S_S + (1-f) \cdot Y \cdot S_S \cdot (1 - e^{-bt})$$

## BOD Associated with Active Biomass

In cases where there are active organisms present, the BOD exerted by the organisms can be calculated from the rate of change in active organisms due to endogenous metabolism, *i.e.,*

$$BOD_{XBH} = (1 - f) \cdot X_{BH} \cdot (1 - e^{-bt}) \quad (24)$$

This must then be added to the soluble and slowly degradable BODs to obtain the total BOD (*i.e.*, sum Eqs. 23, and 24).

## Example

This example demonstrates the BOD calculation procedure for an influent wastewater stream with the following characteristics:

| | |
|---|---|
| $S_T$ | 500 mg COD/L |
| $f_{US}$ | 0.10 |
| $f_{UP}$ | 0.08 |
| $f_{BS}$ | 0.20 |
| $f_{XBH}$ | 0.00 |
| $f_{XSP}$ | 0.75 |

The influent "soluble" and slowly biodegradable concentrations are calculated using the influent fractions:

$$S_{BS} = f_{BS}\, S_T$$

$$= (0.20)(500)$$

$$= 100 \text{ mg COD / L}$$

$$X_S = (1 - f_{US} - f_{UP} - f_{BS} - f_{XBH})\, S_T$$

$$= (1 - 0.10 - 0.08 - 0.20 - 0.0)(500)$$

$$= 310 \text{ mg COD / L}$$

$$X_{SC} = (1 - f_{XSP})\, X_S$$

$$= (1 - 0.75)(310)$$

$$= 77.5 \text{ mg COD / L}$$

$$X_{SP} = (f_{XSP})\, X_S$$

$$= (0.75)(310)$$

$$= 232.5 \text{ mg COD / L}$$

$$S_S = S_{BS} + X_{SC}$$
$$= 100 + 77.5$$
$$= 177.5 \text{ mg COD / L}$$

The soluble $BOD_5$ can then be calculated using Eq.9 and the parameters listed below:

| | |
|---|---|
| *f* | 0.20 |
| Y | 0.666 mg COD/mg COD |
| b | 0.24 $d^{-1}$ |
| k | 0.40 $d^{-1}$ |

Note: The parameter values for *f* and b are for endogenous respiration, and should not be confused with the corresponding terms used in the death-regeneration approach for modeling biomass decay.

$$BOD_S = (1 - Y) \cdot S_S + (1 - f) \cdot Y \cdot S_S \cdot (1 - e^{-b\,t})$$

$$= (1 - 0.666)(177.5) + (1 - 0.20)(0.666)(177.5)(1 - e^{-(0.24)(5)})$$

$$= 125.4 \text{ mg BOD / L}$$

Similarly, the slowly degradable $BOD_5$ can be calculated using Eq. 22.

$$BOD_{XSP} = X_{SP0} \cdot \left[ \left( (1 - Y) + \frac{(1 - f) \cdot b\,Y}{(b - k)} \right) \cdot \left(1 - e^{-k\,t}\right) - \left( \frac{(1 - f) \cdot Yk}{(b - k)} \right) \cdot \left(1 - e^{-b\,t}\right) \right]$$

$$= (232.5) \left[ \begin{array}{l} \left( (1 - 0.666) + \dfrac{(1 - 0.20)(0.24)(0.666)}{(0.24 - 0.40)} \right) \cdot (1 - e^{-(0.40)(5)}) \\ \qquad - \left( \dfrac{(1 - 0.20)(0.666)(0.40)}{(0.24 - 0.40)} \right) \cdot (1 - e^{-(0.24)(5)}) \end{array} \right]$$

$$= 122.9 \text{ mg BOD / L}$$

In this example the active organism fraction is zero, therefore the total $BOD_5$ is the sum of the $BOD_S$ and the $BOD_{XSP}$, *i.e.,*

$$BOD_T = BOD_S + BOD_{XSP}$$
$$= 125.4 + 122.9$$
$$= 248.3 \text{ mg BOD / L}$$

## Effluent BOD

Knowledge of the effluent BOD is useful for quantifying the impact of plant discharges on receiving water bodies, and often is of interest in terms of regulatory requirements and consent limits. Currently BioWin provides information on a number of biodegradable components in any plant output stream (and internal streams). Therefore it is a simple step to quantify both the soluble and total (soluble + particulate) BOD. In BioWin this calculation is based on differing rates of degradation of the different components [e.g. undegraded influent biodegradable material (readily and slowly biodegradable), active organism masses which exert an

endogenous oxygen demand and hence a BOD, etc.]. Essentially BioWin simulates a BOD test for the specified number of days and wastewater composition. This should allow for more accurate estimation of BOD than is provided with models based on the BOD parameter.

## COD *versus* BOD as a Modeling Parameter

The advantage of selecting COD as the parameter for quantifying the "strength" of organic material in the influent, as opposed to BOD or TOC, is that it provides a consistent basis for description of the activated sludge process. Marais and Dold (1985) outlined the rationale which makes COD the appropriate parameter. It is worth reviewing this rationale briefly as selection of the COD parameter is fundamental to the application of the models. Briefly, the suitability of COD is established by considering utilization of organic substrate. In the process of metabolism the organic substrate serves two functions for the organisms as shown schematically in the arrow diagram below:

1. A portion of the organic material is oxidized to $CO_2$ and water, providing energy for maintaining the homeostatic balance for existing cell mass (osmotic pressure, ionic balance, membrane potential, etc.) and for (2) below. The energy is provided by transferring electrons from the organic substrate through the electron transport chain to the terminal electron acceptor (oxygen in the case of an aerobic system, or nitrate under anoxic conditions). Under the substrate limited conditions usually encountered in activated sludge systems the organisms utilize a relatively fixed fraction of the energy available from oxidation for the energy consuming processes.
2. The remaining portion of the organic material is converted into new heterotrophic cell mass, utilizing energy available from process (1).

Regarding the relative proportions allocated between (1) and (2), this is quantified by the ratio:

$$Y_H = \frac{\text{cell mass formed}}{\text{substrate utilized}} \tag{25}$$

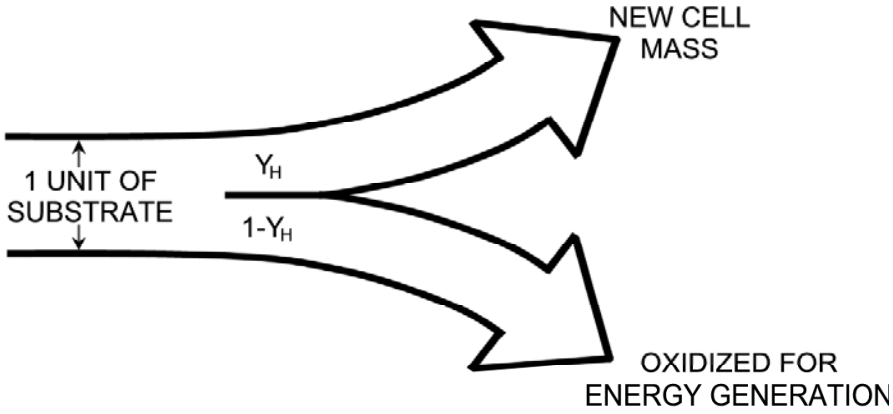
termed the specific yield. From theoretical considerations, under balanced growth conditions the specific yield, in terms of the mass of organisms produced *per electron available for transfer* in the biodegradable organic substrate, should be near constant. This was confirmed by Payne (1970) who reviewed a large number of experimental results for both pure and mixed cultures of heterotrophic organisms. Therefore, if the electron donating potential of the organic substrate in the activated sludge system influent (consisting of a broad spectrum of compounds) is measured, it is possible to quantify sludge production [from $Y_H$] and oxygen demand [from (1 - $Y_H$)]. This observation provides the rationale for selecting the COD parameter.

The electron donating capacity of organic material is measured in the COD test. In the test each mole of oxygen ($O_2$) accepts four electron equivalents ($e^-$ eq); therefore the COD is a direct measure of the electron donating potential. The link between electron equivalents (COD) of the substrate, the near constant yield of organism mass per unit substrate COD, and the corresponding fixed oxygen requirement per unit substrate COD metabolized, make the COD a fundamental parameter in the analysis of activated sludge behavior.

*Regarding the COD of the waste sludge, this may be measured directly by the COD test or may be estimated from the VSS measurement. Because cell mass has an approximately constant composition and is made up of an essentially fixed number of electron equivalents (e- eq) per unit mass, the COD/VSS ratio is near constant (approximately 1.48 mgCOD/mgVSS).*

A factor which adds impetus to the selection is that mass balances can be made in terms of COD. As electrons cannot be created or destroyed, in a biosystem operated at steady state the mass of COD entering with the influent per unit time must equal the sum of (1) the mass of COD leaving in the effluent, (2) the COD of the wasted sludge, and (3) the oxygen (or oxygen equivalent) consumed in the utilization of the organic material (from the oxygen utilization rate measurement); that is, a mass balance is possible.

Characteristics of the COD as a measure of the "strength" of a wastewater are not realized by either the BOD or the TOC parameters. The BOD measures only that portion of the $e^-$ eq in the substrate utilized for energy generation and excludes the portion of the substrate $e^-$ eq transformed into new cell mass. Therefore BOD cannot be used as the basis for a mass balance. The TOC is deficient in that the ratio of carbon/$e^-$ eq differs between organic compounds and therefore TOC is an inappropriate parameter when dealing with the mixed substrate influents to wastewater treatment plants.




*Schematic representation of the utilization of substrate by heterotrophic organisms showing the division between substrate oxidized for energy generation and growth of new cell mass.*

**Note:** The user must specify influent concentrations in terms of COD; however, the simulator can estimate the soluble and total BOD for any input element, process unit, or stream. The user may specify the time basis for the BOD calculation (5, 7, or 20 days).