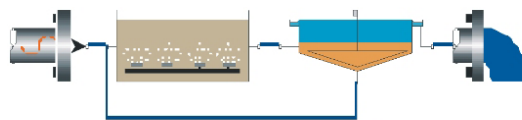


BIOWIN 2.1

Created by process engineers...for process engineers.

RELEASE NOTES FOR BIOWIN 2.1



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CHAPTER 1 : OVERVIEW OF NEW DEVELOPMENTS

The new **Full Plant Edition** is a significant step for BioWin, and an advancement in the modeling of wastewater treatment plants. BioWin tracks more organic and inorganic components than any other simulator, and allows a complete mass balance for recycled sidestreams and supernatants. The simulator now includes accurate pH modeling and the effect of pH on biological and chemical processes. The integrated process model in BioWin works for any environmental condition, whether in aerated or un-aerated activated sludge tanks, fermenters, or digesters. This allows seamless integration of the processes in the whole plant.

In this document:

- Chapter 1 provides an overview of changes in BioWin 2.1.
- Chapter 2 briefly describes new functionality in the interface.
- Chapter 3 introduces the enhanced modeling features.
- Chapter 4 summarizes state variables and model parameters, showing additions and any changes to default values.

1.1 NEW MODELING CAPABILITIES

- BioWin 2.1 comes with a new set of default parameters, which have been calibrated on hundreds of wastewater treatment plants. These parameters (such as the new nitrification defaults) reflect results from new research and measurement methods.
- EnviroSim has developed the first plant-wide pH model using a unique method based on the dissociation state of the phosphate, carbonate, ammonium and volatile organic acid systems, concentrations of strong acids and bases, chemical precipitation reactions, and stripping of components such as ammonia and carbon dioxide. Process rates are affected by pH instead of alkalinity.
- The pH model allows prediction of struvite and calcium phosphate formation in various units around the plant, and more accurate simulation of the fate of phosphate. Magnesium and potassium uptake and release in digesters is simulated with biological phosphorus removal.
- The new chemical phosphorus removal module simulates alum or ferric dosing for phosphorus precipitation and chemical sludge formation integrated with the biological model. The precipitation reactions are pH-dependent.
- EnviroSim has significantly improved modeling of denitrification with methanol addition. BioWin contains a methanol-specific biomass that simulates adaptation to startup of methanol dosing, minimum anoxic SRT, and substrate specific anoxic yields.

- The enhanced integrated digester model describes the acidogenic (prefermenters) and methanogenic phases, predicts gas flow/composition (methane, carbon dioxide and hydrogen) and pH.
- Surface aerators and brushes have been added to our aeration model.
- Membranes in membrane bioreactors and various sludge thickening devices can now be simulated with a volumeless phase separation unit – the point settler.
- BioWin provides the most detailed modeling of inert inorganic suspended solids available: influent inerts, spontaneously forming precipitates, chemical sludge from phosphorus removal and biomass stored inert inorganics are all accounted for.
- We have significantly improved plant-wide N and P balances. BioWin now tracks 45 components and 20 ion species.
- The International Modeling Kit includes standard models such as the ASM series (ASM1, ASM2d, ASM3) and the double-exponential settler model. The Model Builder enables users to customize models or to create their own – starting from scratch or by modifying existing models.

1.2 ENHANCED USABILITY

- The BioWin Manual has been completely revised and updated, and contains close to 700 pages of modeling guidance, useful help, hints and tips for the simulator user.
- BioWin now contains a Configuration Cabinet. Users can load typical process configurations directly from the cabinet and use them in their own projects or for demonstration/learning.
- The BioWin Album received a significant update with more features, a Chart Master and Chart annotation tools. The new Chart Master allows you to automatically format multiple charts easily in the BioWin Album. BioWin comes with four different chart templates, and users also can create their own.
- It is easier to find information in BioWin than ever. Key variables for each process (OUR, Nitrate Production Rate, Specific Denitrification Rate, etc.) are readily accessible. The Summary Panes below the drawing board were updated to display the most relevant information. Pointing at pipes now reveals information on flow, concentration, and mass rates of their streams. A sludge output element is available that provides information on sludge composition. Mass balances for COD, N and P and process rates are available in each element.
- Multiple SRT calculators can be defined in the plant configuration. For example a full plant SRT, anoxic SRT or different SRTs for different process trains can be all set up. The SRT can be plotted as it changes during a dynamic simulation.
- Sludge blanket height is estimated and can be plotted in model clarifiers.
- The choice of either full or abbreviated names for state variables and other parameters is available.
- Existing BioWin32 configurations are automatically updated upon loading into BioWin 2.1.
- An Influent Specifier is available for BioWin to aid with establishing influent fractions based on typically measured parameters, such as TSS and BOD.
- Other improvements include floating/docking toolbars, enhancements to the Report to Word™ feature, autosaving dynamic simulations as they progress, unmonitoring of parameters, improved numerical procedures for the steady state solver, and other improvements and fixes.

CHAPTER 2 : CHANGES TO THE INTERFACE

2.1 THE INTERFACE

The BioWin interface has changed, and the shortcuts displayed on the menu bar change, depending on which tab is selected.

- **Main tab** : Simulations are run from the **Main** tab.
- **Configure tab** : The **Configure** tab is selected when setting up a system.
- **Calculator tab** : Several SRT calculators can be configured via the **Calculators** tab. The one designated as the 'active' SRT is displayed on the status bar at the bottom of the screen.

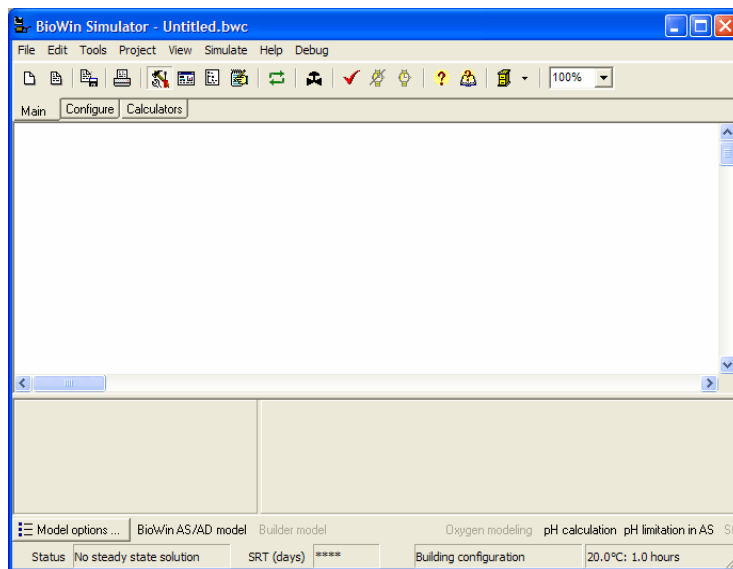


FIGURE 2.1. THE BIOWIN INTERFACE.

A useful feature added to the interface is that information on streams (flow, concentration and mass rate) is displayed in the lower right pane when you point at pipes:

Name: Pipe15		Type: Pipe
Flow of 2.00 ML/d from WAS splitter		
Variable	Concentration mg/L	Mass rate kg/d
TCOD	8785.80	17571.60
TCBOD	2846.75	5693.51
TKN	503.87	1007.74
TP	306.87	613.73
VSS	5923.28	11846.55
TSS	7956.89	15913.77

BioWin is installed with a number of pre-configured systems (and Albums). These can be accessed from the Cabinet button.

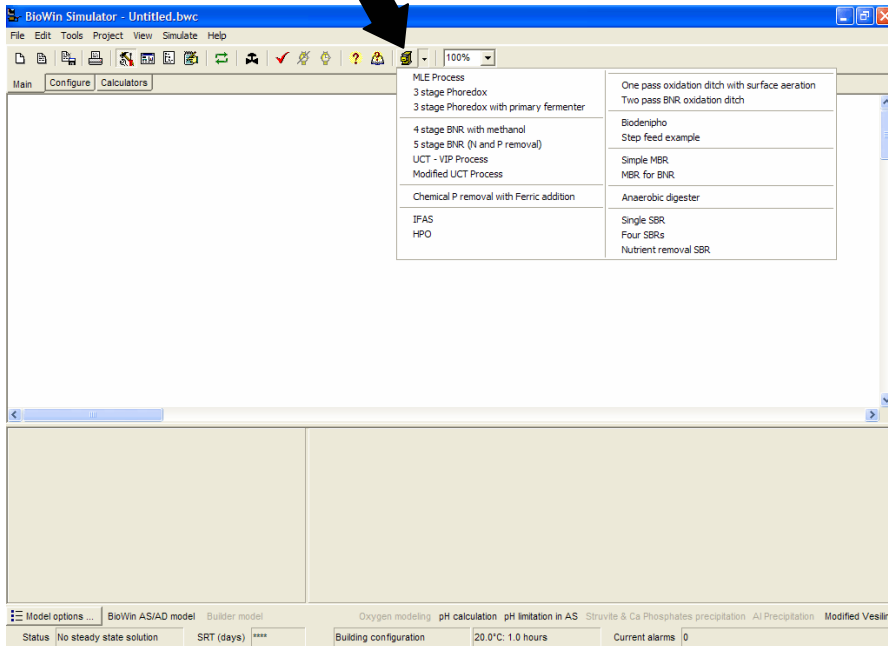


FIGURE 2.2. OPENING THE CABINET PROVIDES A NUMBER OF PRE-CONFIGURED SYSTEMS.

2.2 NEW ELEMENTS IN BIOWIN

A number of new elements have been included:

- **Methanol input**

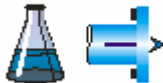
Methanol



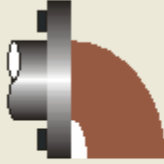
A methanol input was available in BioWin32. However, a specific methanol-utilizing biomass, Z_{BMETH} , has been included in the model.

- **Metal addition input** (for ferric or alum addition)

Metal addition



- **Sludge output**



Concentrations		Flow	2.00 ML/d
	TSS		0.8 %
	VSS as % of TSS		74.44 %
	N as % of TSS		6.49 %
	P as % of TSS		3.86 %
Mass flows		pH	6.81
	TSS		15913.77 kg/d
	VSS		11846.55 kg/d

- **Brush aerator bioreactor**

Bioreactor (brush aerators)



- **Surface aerator bioreactor**

Bioreactor (surface aerators)



- **General mixer** (for combining multiple streams)



- **Point clarifier**



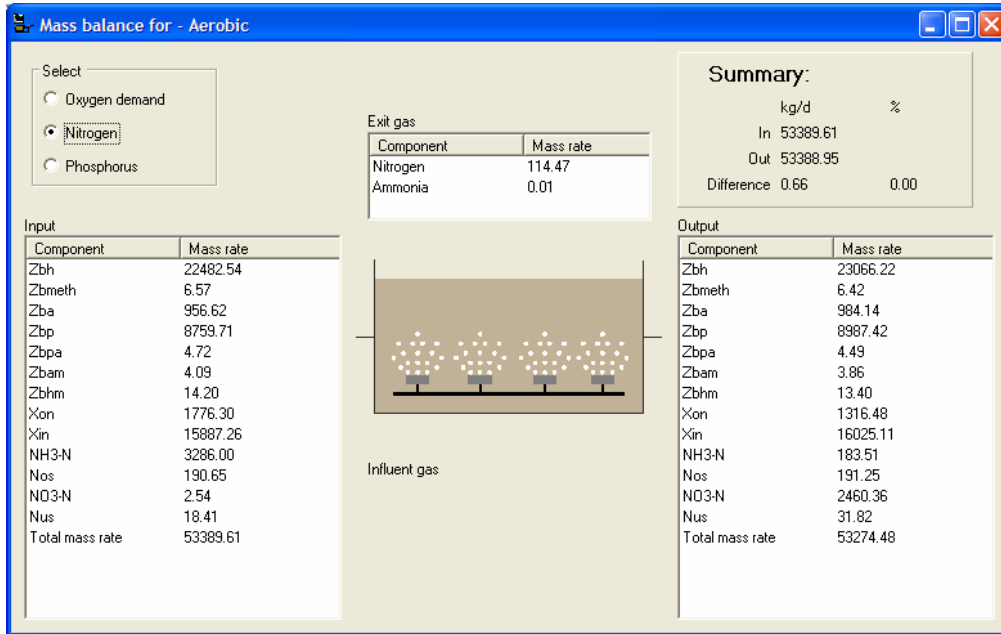
This phase separation element is a simplification of the ideal settler - it has no volume. Fractional solids removal is applied and the remaining solids are instantly returned in the underflow.

Typical uses for this element:

- Membrane bioreactors.
- Dewatering units and other phase separation elements that contain a negligible volume of sludge (much faster run time compared to the dewatering unit with volume in Version 1.2. In 2.1 dewatering units have no volume either).
- Simple simulations (faster model than the ideal settler, but ignores sludge volume).
- Verifying simulations done in other packages or using international standard models (SSSP, and the ASM model set).

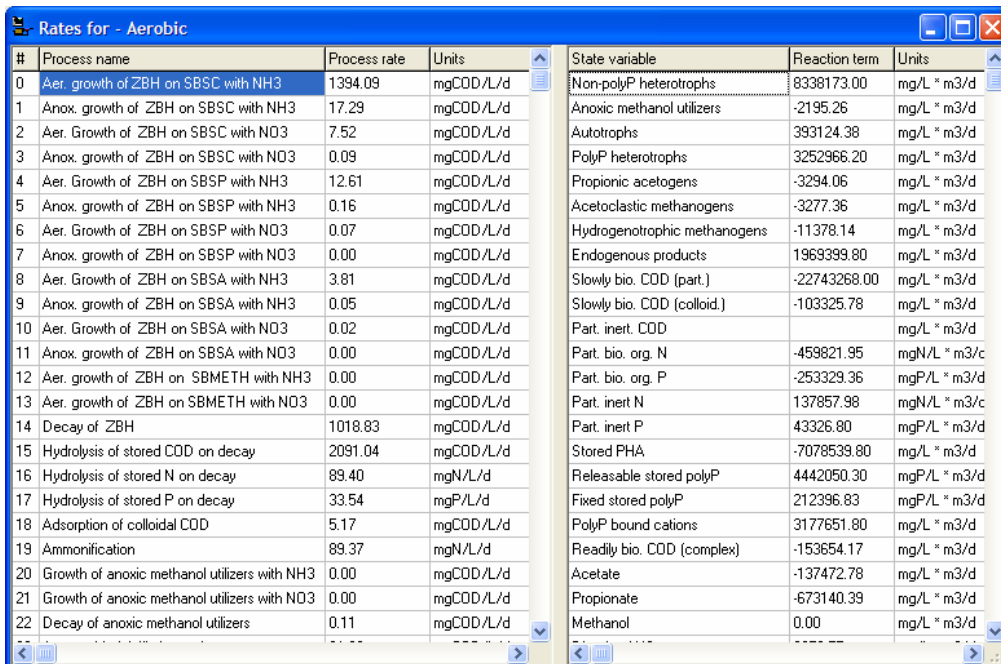
2.3 MASS BALANCE INFORMATION ON SPECIFIC ELEMENTS

Right click on an element, and select the Mass Balance option.



2.4 KINETIC/RATE INFORMATION ON SPECIFIC ELEMENTS

Right click on an element, and select the Rates option.



Rates for - Aerobic

#	Process name	Process rate	Units	State variable	Reaction term	Units
0	Aer. growth of ZBH on SBSC with NH3	1394.09	mgCOD/L/d	Non-polyP heterotrophs	8338173.00	mg/L * m3/d
1	Anox. growth of ZBH on SBSC with NH3	17.29	mgCOD/L/d	Anoxic methanol utilizers	-2195.26	mg/L * m3/d
2	Aer. Growth of ZBH on SBSC with NO3	7.52	mgCOD/L/d	Autotrophs	393124.38	mg/L * m3/d
3	Anox. growth of ZBH on SBSC with NO3	0.09	mgCOD/L/d	PolyP heterotrophs	3252966.20	mg/L * m3/d
4	Aer. Growth of ZBH on SBSP with NH3	12.61	mgCOD/L/d	Propionic acetogens	-3294.06	mg/L * m3/d
5	Anox. growth of ZBH on SBSP with NH3	0.16	mgCOD/L/d	Acetoclastic methanogens	-3277.36	mg/L * m3/d
6	Aer. Growth of ZBH on SBSP with NO3	0.07	mgCOD/L/d	Hydrogenotrophic methanogens	-11378.14	mg/L * m3/d
7	Anox. growth of ZBH on SBSP with NO3	0.00	mgCOD/L/d	Endogenous products	1969399.80	mg/L * m3/d
8	Aer. Growth of ZBH on SBSA with NH3	3.81	mgCOD/L/d	Slowly bio. COD (part.)	-22743268.00	mg/L * m3/d
9	Anox. growth of ZBH on SBSA with NH3	0.05	mgCOD/L/d	Slowly bio. COD (colloid.)	-103325.78	mg/L * m3/d
10	Aer. Growth of ZBH on SBSA with NO3	0.02	mgCOD/L/d	Part. inert. COD		mg/L * m3/d
11	Anox. growth of ZBH on SBSA with NO3	0.00	mgCOD/L/d	Part. bio. org. N	-459821.95	mgN/L * m3/c
12	Aer. growth of ZBH on SBMETH with NH3	0.00	mgCOD/L/d	Part. bio. org. P	-253329.36	mgP/L * m3/d
13	Aer. growth of ZBH on SBMETH with NO3	0.00	mgCOD/L/d	Part. inert N	137857.98	mgN/L * m3/c
14	Decay of ZBH	1018.83	mgCOD/L/d	Part. inert P	43326.80	mgP/L * m3/d
15	Hydrolysis of stored COD on decay	2091.04	mgCOD/L/d	Stored PHA	-7078539.80	mg/L * m3/d
16	Hydrolysis of stored N on decay	89.40	mgN/L/d	Releasable stored polyP	4442050.30	mgP/L * m3/d
17	Hydrolysis of stored P on decay	33.54	mgP/L/d	Fixed stored polyP	212396.83	mgP/L * m3/d
18	Adsorption of colloidal COD	5.17	mgCOD/L/d	PolyP bound cations	3177651.80	mg/L * m3/d
19	Ammonification	89.37	mgN/L/d	Readily bio. COD (complex)	-153654.17	mg/L * m3/d
20	Growth of anoxic methanol utilizers with NH3	0.00	mgCOD/L/d	Acetate	-137472.78	mg/L * m3/d
21	Growth of anoxic methanol utilizers with NO3	0.00	mgCOD/L/d	Propionate	-673140.39	mg/L * m3/d
22	Decay of anoxic methanol utilizers	0.11	mgCOD/L/d	Methanol	0.00	mg/L * m3/d

2.5 CUSTOMIZING BIOWIN

Various features can be customized via the **Tools/Customize** and **Tools/New Project Options** menu. For example, you can select to display either full names or abbreviated (cryptic) descriptions for the many parameters. These selections are persistent once BioWin is restarted.

Certain features can also be customized for the current project via the **Project/Current Project Options** menu.

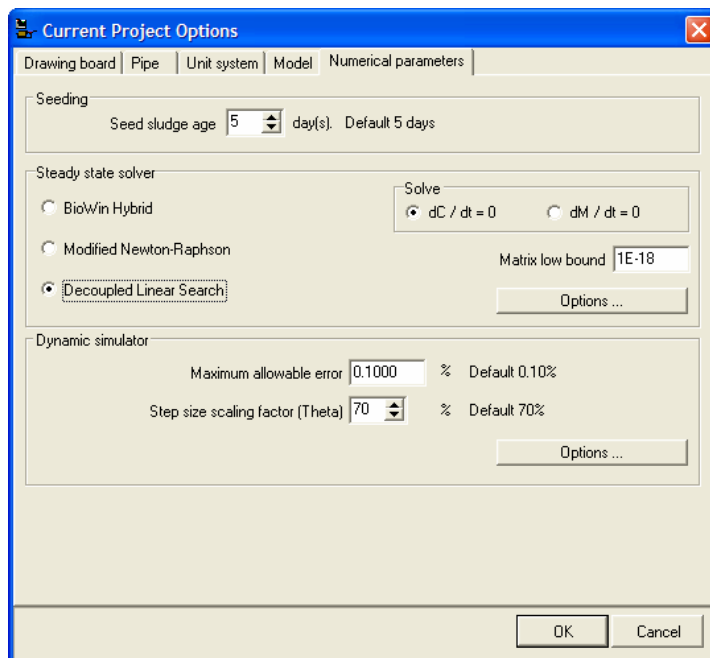
2.6 NUMERICAL SOLVER SETTINGS

The solver for steady state simulations has been refined. The default solver (BioWin Hybrid) uses a combination of Newton-Raphson and Decoupled Linear Search (DLS) numerical methods. Typically steady state solutions are found in 5 to 12 iterations. Nevertheless, with certain configurations the solver may encounter difficulties in converging to a solution. The on-line Help and the printed manual include a section on **Managing BioWin Projects/ Numerical parameters/ Tips for systems that are difficult to solve**.

Four approaches for resolving problem situations are suggested below.

2.6.1 DECOUPLED LINEAR SEARCH

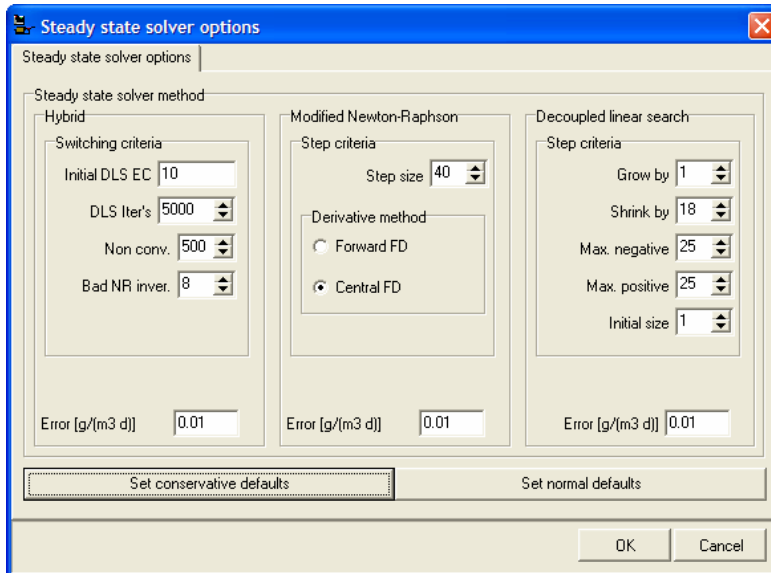
For very large systems (particularly those including multiple model clarifier units) try selecting the **Decoupled linear search** solver via the **Project/Current Project Options/ Numerical parameters** menu.



2.6.2 CONSERVATIVE SOLVER SETTINGS

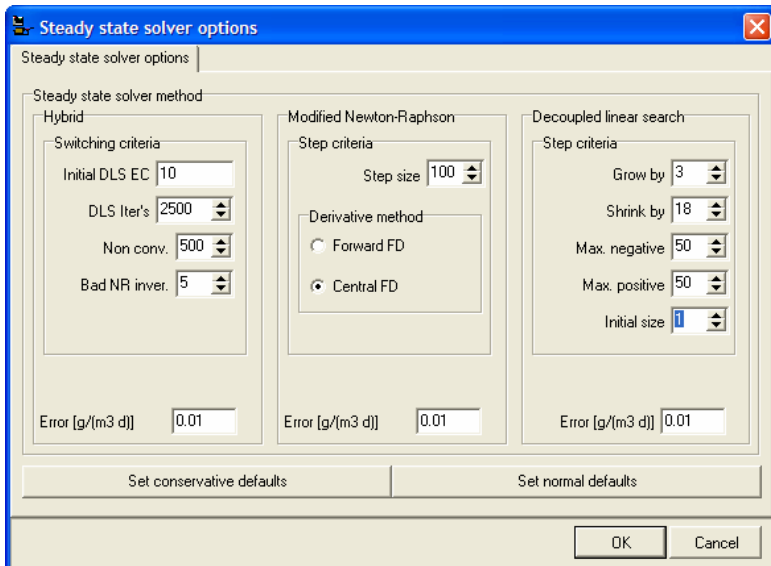
If the Error value displayed in the **Steady state analysis** window does not decrease from iteration to iteration after say 15 or 20 iterations, try selecting conservative solver settings. From the **Project/Current Project Options/ Numerical parameters** menu, click on the **Options** button in the **Steady state solver**

method section, and click on the **Set conservative defaults** button. This change may result in slow solver convergence, but often will improve solver stability (the Error value should decrease from iteration to iteration).



2.6.3 ADJUSTING DLS SOLVER INITIAL SIZE

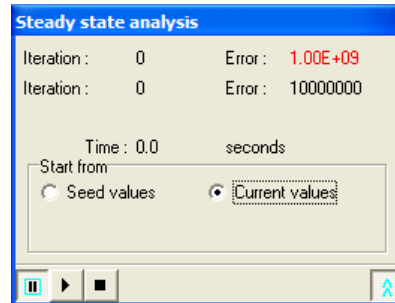
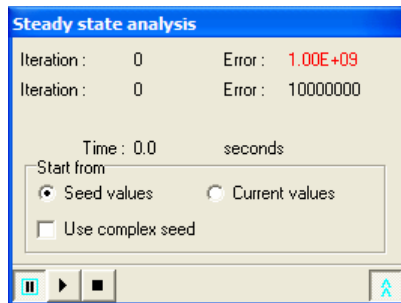
For systems with very high recycle flow rates (e.g. oxidation ditch systems) or systems with 'recycles-within-recycles', try adjusting one DLS solver setting as follows. From the **Project/Current Project Options/ Numerical parameters** menu, click on the **Options** button in the **Steady state solver method** section, and change the **Initial size** in the **Decoupled linear search** section to 1 (from the default value of 5).



2.6.4 TWO-STEP STEADY STATE SOLUTION

If it appears that the solver is encountering problems with pH calculations (e.g. pH values in units oscillate significantly from iteration to iteration), a two-step approach may resolve the problem. From the

Project/Current Project Options/ Model menu (or by clicking on the **Model options** button), de-select (uncheck) the **Include pH calculations** option. Run the steady state solver, starting from **Seed values**. This should converge to a solution (with pH 7 in all units). Return to the **Model options** and select (check) the **Include pH calculations** option. Re-run the steady state solver, but start from **Current values**.



CHAPTER 3 : NEW MODEL FEATURES

3.1 PH MODELING

pH plays a fundamental role in all biological processes, including the activated sludge and anaerobic digestion process. Due to the complexity of calculating pH in wastewater, BioWin previously used alkalinity as an indicator for pH instability. If alkalinity is low, there is a potential for rapid pH changes. However, this is a weak correlation and does not account for high pH inhibition.

A general pH model has been implemented in Version 2.1 to include all of the major acid-base systems and strong ions typically found in municipal wastewaters. The objective of the model is to calculate the pH throughout the activated sludge plant, including the liquid and solids lines.

Some developments made possible as a result of the ability to model pH are:

- Gas phase modeling which is important for modeling anaerobic digestion and precipitation processes. Calculation of gas transfer rates (e.g. CO₂ and ammonia) requires knowledge of the species ionization states and consequently the pH of the system.
- Inhibition of biological activity at low and high pH.
- pH dependent equilibrium modeling of aluminum and ferric dosing for phosphorus precipitation, including hydroxide sludge formation.
- pH dependent modeling of the spontaneous precipitation of struvite and calcium phosphates, integrated into the biological model matrix. Accurate prediction of struvite precipitation also requires modeling of magnesium concentrations, both the soluble magnesium and that stored in organisms.

The equilibrium part of the pH model does not have parameters to calibrate, as ionization constants are known from literature. An estimation of CO₂ mass transfer coefficient is required, using the same area for transfer as in the existing oxygen transfer model.

3.2 CHEMICAL P PRECIPITATION (FERRIC/ALUM)

Chemical precipitation of phosphorus with ferric salts or alum addition is included in the model. Either ferric or aluminum phosphate precipitation can be selected as an option, but not both simultaneously.

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}H₂PO₄OH_{3.8} or Al_{0.8}H₂PO₄OH_{1.4}), a soluble metal-phosphate complex (FeH₂PO₄²⁺ or AlHPO₄⁺), 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 (PO₄³⁻, HPO₄²⁻, H₂PO₄⁻, H₃PO₄). 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 the case of a large metal overdose, the figure below demonstrates the residual soluble phosphorus species concentration dependence on pH.

3.3 STRUVITE, HDP AND HAP PRECIPITATION

The model incorporates reactions for spontaneous precipitation of struvite, HDP (hydroxy-dicalcium-phosphate – $\text{Ca}_2\text{HPO}_4(\text{OH})_2$) and HAP (hydroxy-apatite – $\text{Ca}_5(\text{PO}_4)_2\text{OH}$). BioWin is based on an integrated activated sludge – anaerobic digestion model (ASDM) that has been extended with water chemistry, simulation of pH, and various chemical reactions. Formation of struvite usually occurs in digesters or in output streams from digesters (particularly if there is an increase in pH). Necessary requirements for the formation of struvite are the presence of magnesium, ammonium and phosphate ions at a pH favoring precipitation. These conditions typically are encountered in the digestion of waste sludge from a biological phosphorus removal system. For example:

1. **Magnesium, ammonia and phosphorus uptake in the bio-P process:** The model predicts phosphorus uptake and storage as polyphosphate (poly-P) and release in anaerobic, anoxic and aerobic activated sludge reactors. Along with the formation of poly-P, magnesium and other charge balancing cations are stored in the biomass according to an experimentally determined stoichiometric ratio. Assimilation of nitrogen is based primarily on the N content of biomass. The biomass containing stored phosphorus and cations (including magnesium), as well as nitrogen is removed from the activated sludge process through wasting and is directed to the anaerobic digester unit.
2. **Transport to the digester:** The integrated ASDM is based on a single model matrix; therefore continuity and mass balances on Mg, N, P and all other components are automatically maintained.
3. **Release of magnesium, ammonia and phosphorus in the digester:** Anaerobic degradation processes are included in the ‘four population’ anaerobic digestion model. These result in the release of phosphate, cations associated with polyP (including magnesium), and organic nitrogen which is converted to ammonia.
4. **Weak acid-base system in the digester:** The equilibrium based pH model accounts for the various species in the digester (phosphates, carbonates, ammonia, nitrate, acetate, propionate, calcium, magnesium and other strong acids and bases), as well as gas transfer for CO_2 and ammonia. This module calculates the current pH and pH changes in the digester (and other parts of the plant).
5. **Struvite formation:** Struvite precipitation is described according to the solubility equation from equilibrium chemistry [the implementation is kinetic for numerical reasons, extended from Musvoto *et al.*, (2000)]. This process is sensitive to pH because this impacts the ammonia and phosphate speciation. The equilibrium solubility equation is as follows:



3.4 GAS PHASE MODELING

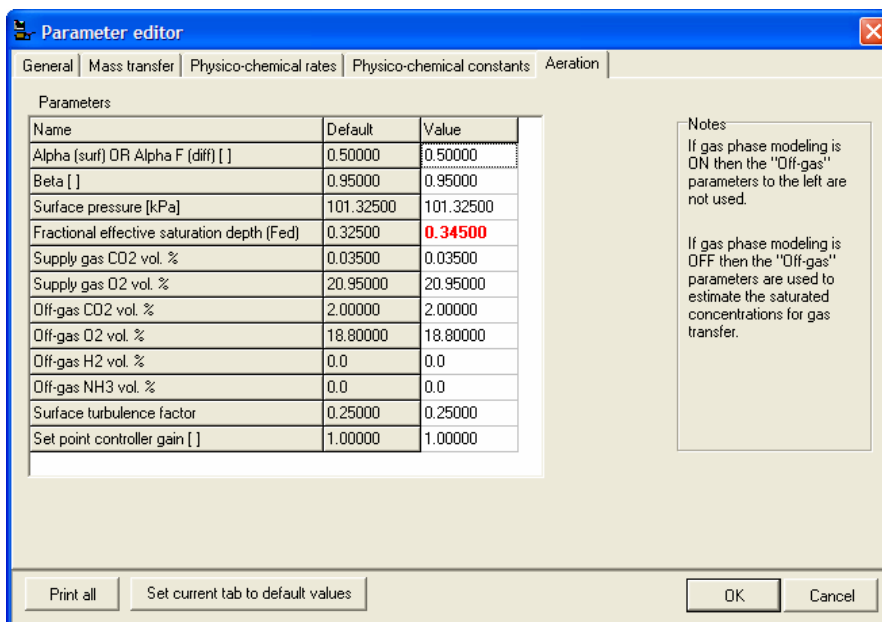
BioWin 2.1 introduces modeling of the gas phase composition (i.e. modeling of the gas phase concentrations).

BioWin considers six different gases: oxygen (O_2), carbon dioxide (CO_2), ammonia (NH_3), hydrogen (H_2), nitrogen (N_2) and methane (CH_4). Nitrogen and methane are considered insoluble so any production of these gases is immediately reported in the gas phase, and no mass transfer limitations between the phases is

considered. Mass transfer considerations govern the transfer between liquid and gas phases for the remaining four gases.

The composition of gas phase is critical in determining the pH in anaerobic digesters, as the carbon dioxide content in the digester gas phase strongly influences the dissolved carbon dioxide concentration in the liquid phase. Knowledge of the gas phase concentration is also important in determining gas production rates. In anaerobic digesters the composition of the gas phase is always modeled

In other aerated processes (bioreactors, aerobic digesters, SBRs) the exit gas composition usually is quite uniform. In these units, if gas phase modeling is switched off (the default), the exit gas composition is assumed fixed. In this case, the off-gas composition is specified in the **Parameters / Other / Aeration** tab (see below). The default values are typical for bioreactor off-gas composition. These values are used to determine the liquid phase saturation concentration for each component (e.g. saturation DO, which impacts oxygen transfer behavior). Those saturation concentrations are used as the basis for modeling mass transfer of gases between the liquid and gas phases.



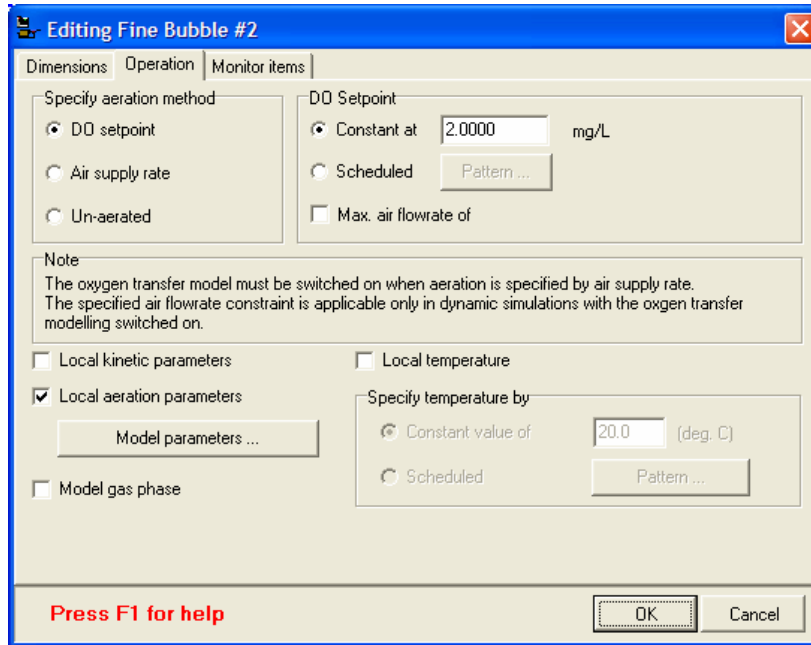
In certain circumstances the gas phase composition may differ from the values specified above; for example, when there are significant changes in influent load or pH. The difference may influence pH and oxygen transfer (because the oxygen content of the air changes during aeration). The user may elect to model the gas phase by selecting **Model gas phase** on the **Element-Properties-Operation** tab (see below). In this case BioWin simulates the change in gas phase composition, and the impact this has on factors such as DO saturation concentration, oxygen transfer, pH, etc. [The default setting is off in which case BioWin uses the "off-gas" concentrations specified in the **Aeration** parameters tab as described above].

For surface aerators, BioWin uses the "Supply gas" concentrations to determine the saturation concentration.

Gas phase modeling in aerated reactors slows down the simulation and is not usually required. There are a few reasons to activate gas phase modeling:

- Detailed pH simulation or oxygen transfer studies.
- Variable loading may result in changes in the "off-gas" composition during simulations.

- Unusual pH conditions may result in stripping and consequently variable gas phase composition.
- Off-gas concentrations vary or differ significantly from the typical defaults supplied in Project-Parameters-Other-Aeration Tab.
- Best achievable model accuracy is required.



3.5 ASH CONTENT OF BIOMASS

In systems with synthetic wastewater influents such as glucose the MLSS typically is slightly higher than the MLVSS even though the influent contains no ISS. Presumably this is due to the inclusion of some dissolved inorganic salts within the organism in the growth process. To account for this situation, BioWin now allows an ash content for biomass (and endogenous residue) to be specified via the **Project / Parameters / Other / General** tab.

Note: When loading 'old' BioWin files, the value for ash content is set at zero. When new configurations are started the value is set to the default of 8%.

Consider the system shown below. Run a steady state simulation and open the Album (see below). The difference between TSS and VSS is 9.14 mg/L. There is no influent ISS, so this difference must be accounted for as synthesis ISS. The sum of the biomass components (heterotrophs, autotrophs and endogenous residue in this case) is: $98.24 + 2.62 + 48.45 = 149.31$ mgCOD/L. All these components have COD/VSS ratios of 1.42, so the corresponding VSS contribution from biomass is $149.31/1.42 = 105.14$ mgVSS/L.

In this case the synthesis ash content was specified as 8%; that is, if X is the ash content in mg/L:

$$\frac{X}{105.14 + X} = 0.08$$

Solving: $X = 9.14$ mg/L

Elements (Conc.)	VSS [mgVSS/L]	TSS [mgTSS/L]	SCat [mg/L]	SAn [mg/L]	Zbh [mg/L]	Zba [mg/L]	Zbp [mg/L]	Ze [mg/L]
COD Influent	0.00	0.00	5.00	10.77	0.00	0.00	0.00	0.00
Bioreactor	106.53	115.67	4.88	10.64	98.24	2.62	0.00	48.45
Effluent	106.53	115.67	4.88	10.64	98.24	2.62	0.00	48.45

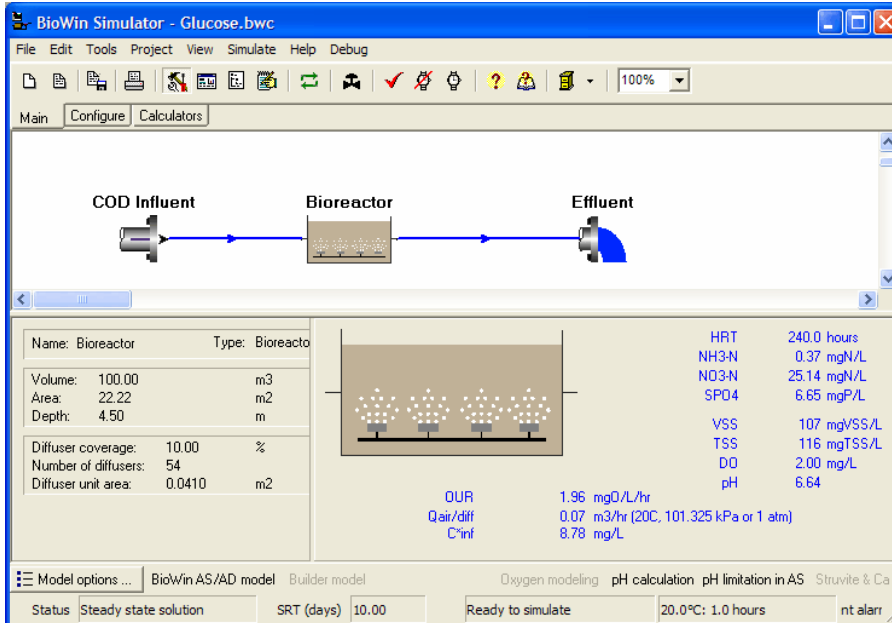
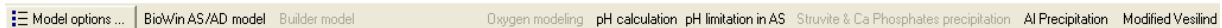


FIGURE 3.1. EXAMPLE DEMONSTRATING ASH CONTENT OF BIOMASS.

3.6 SELECTING MODEL OPTIONS

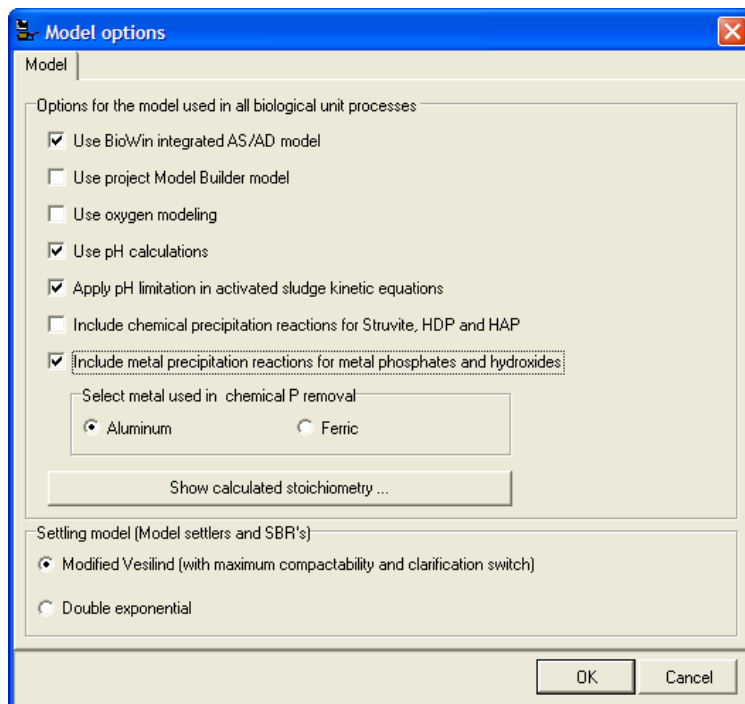
Model options can be switched on and off as required for a specific system. For example, if no ferric salts or alum are added to a particular system, then there is no necessity to include simulation of this model component. The current status of the selected model options is displayed in a bar along the bottom of the screen immediately above the status bar.



Clicking on the **Model options** button on the left opens a dialog where the user can switch options on and off:

- **BioWin integrated AS/AD model:** This is the default activated sludge and anaerobic digestion biological model.
- **Project Model Builder model:** This option is selected if (a) an add-on to the BioWin model is to be included, or (b) if the BioWin integrated AS/AD model is to be replaced by an alternative model such as ASM1, ASM2d or ASM3.

- **Oxygen modeling:** If this option is **not** selected, it is assumed that there is an immediate response to DO setpoint changes (i.e. without a lag in response). Whether this option is on or off, within bioreactors BioWin accounts for additional aeration requirements to raise the DO of input streams to the reactor DO.
- **pH calculations:** pH in all units and streams is calculated when this option is selected; otherwise pH 7 is assumed (pH in digesters can be specified separately).
- **Apply pH limitation in activated sludge kinetic equations:** pH dependency of activated sludge kinetic equations is accounted for when this option is selected. In anaerobic digesters pH dependency is always applied.
- **Chemical precipitation reactions for Struvite, HDP and HAP:** This option must be selected to model potential precipitation of struvite ($\text{MgNH}_4\text{PO}_4 \cdot 6\text{H}_2\text{O}$), HDP (hydroxy-dicalcium-phosphate – $\text{Ca}_2\text{HPO}_4(\text{OH})_2$) and HAP (hydroxy-apatite – $\text{Ca}_5(\text{PO}_4)_2\text{OH}$). pH calculations must be selected.
- **Metal precipitation reactions for metal phosphates and hydroxides:** This option should be selected for chemical phosphorus precipitation with ferric or alum addition. pH calculations must be selected.
- **Settling model (applied in model settlers and SBRs):** The modified Vesilind (maximum compactability and clarification switch) or the Double Exponential model can be selected.



CHAPTER 4 : STATE VARIABLES AND MODEL PARAMETERS

The modeling capabilities in BioWin have been expanded considerably. In the new version:

- The activated sludge / anaerobic digestion biological model has been extended. For example, a separate population of methanol utilizing heterotrophs has been included.
- pH modeling has been integrated.
- Chemical phosphorus precipitation with ferric salts or alum addition has been incorporated.
- Struvite, HDP and HAP precipitation can be modeled.

Many new state variables and model parameters have been added. This section summarizes changes and additions to state variables and model parameters.

4.1 STATE VARIABLES

The table below summarizes **changes to state variables in Version 2.1 compared to Version 1.2 (IN RED)** and **additions of new state variables (IN BLUE)**.

TABLE 4.1. STATE VARIABLES IN BIOWIN 2.

Cryptic (short) name	Full descriptive name	Unit	Note
Z _{BH}	Non-polyP heterotrophs	mgCOD/L	
S _{BSC}	Readily biodegradable complex COD (non-VFA)	mgCOD/L	
S _{BSP}	Propionate	mgCOD/L	
S _{BSA}	Acetate	mgCOD/L	
S _{US}	Soluble inert COD	mgCOD/L	
X _{SC}	Slowly biodegradable colloidal COD	mgCOD/L	
X _{SP}	Slowly biodegradable particulate COD	mgCOD/L	
X _I	Particulate inert COD	mgCOD/L	
Z _E	Endogenous products	mgCOD/L	
DO	Dissolved oxygen	mgO ₂ /L	
Z _{BMETH}	Anoxic methanol utilizers	mgCOD/L	
S _{BMETH}	Methanol	mgCOD/L	
Z _{BA}	Autotrophs	mgCOD/L	
X _{ON}	Particulate biodegradable organic nitrogen	mgN/L	

N _{OS}	Soluble biodegradable organic nitrogen	mgN/L	
X _{IN}	Particulate inert organic nitrogen	mgN/L	
N _{US}	Soluble inert organic nitrogen	mgN/L	
NH ₃ -N	Ammonia N	mgN/L	
NO ₃ -N	Nitrate N	mgN/L	
Z _{BP}	PolyP heterotrophs	mgCOD/L	
S _{PHB}	Stored PHA	mgCOD/L	
PO ₄ -P (incl. Me)	PO ₄ (including Metal complexed)	mgP/L	All PO ₄ even if metal complexed
X _{OP}	Particulate biodegradable organic phosphorus	mgP/L	
X _{IP}	Particulate inert organic phosphorus	mgP/L	
PP _{-LO}	Releasable stored polyP	mgP/L	
PP _{-HI}	Fixed stored polyP	mgP/L	
Z _{BPA}	Propionic acetogens	mgCOD/L	
Z _{BAM}	Acetoclastic methanogens	mgCOD/L	
Z _{BHM}	Hydrogenotrophic methanogens	mgCOD/L	
S _{BH2}	Dissolved H ₂	mgCOD/L	
ISS	Influent inorganic suspended solids	mgTSS/L	
S _{Mg}	Soluble magnesium	mgMg/L	
X _{STRU}	Precipitated struvite	mgTSS/L	
X _{Cat}	Biologically stored Cations	mgTSS/L	
S _{Ca}	Soluble calcium	mgCa/L	
X _{HDP}	Hydroxy-dicalcium-phosphate	mgTSS/L	
X _{HAP}	Hydroxy-apatite	mgTSS/L	
S _{Me}	Dissolved and complexed metal	mgMe/L	Fe ³⁺ or Al ³⁺
S _{CO2t}	Total CO ₂ (inorganic carbon)	mmol/L	
S _{CAT}	Cations (strong bases)	meq/L	K ⁺ and others
S _{AN}	Anions (strong acids)	meq/L	Cl ⁻ and others
S _{UD1}	User-defined variable 1	mgCOD/L	Soluble, COD
S _{UD2}	User-defined variable 2	mgCOD/L	Soluble, COD
X _{UD1}	User-defined variable 3	mgVSS/L	Particulate, VSS
X _{UD2}	User-defined variable 4	mgTSS/L	Particulate, TSS
ALK	Alkalinity	meq/L	Not a state variable in 2.1; calculated from equilibrium chemistry

4.2 MODEL PARAMETER CHANGES

The tables below summarize **changes to values of default parameters in Version 2.1 compared to Version 1.2 (IN RED)** and **additions of new parameters with their default values (IN BLUE)**.

The main changes (**IN RED**) are with respect to the nitrification kinetic and stoichiometric model parameters. The basis for these changes is outlined in a recent WERF report (WERF, 2003) – see below. BioWin users are strongly encouraged to obtain this report (copies can be ordered at www.werf.org) because it contains a wealth of information on modeling and simulation.

WERF (Water Environment Research Foundation) (2003) **Methods for wastewater characterization in activated sludge modeling**. Project 99-WWF-3, ISBN 1-893664-71-6. Alexandria, Virginia.

4.2.1 KINETIC PARAMETERS

TABLE 4.2. KINETIC PARAMETERS IN BIOWIN 2.

Autotrophs	New Default	Old Default	New Arrhenius	Old Arrhenius
Max. spec. growth rate	0.900	0.500	1.072	1.096
Substrate (NH ₄) half sat.	0.700	1.000	1.000	1.000
Aerobic decay rate	0.170	0.040	1.029	1.029
Anoxic/anaerobic decay rate	0.080		1.029	
CO ₂ half sat. for autotrophs	0.010		1.000	

Heterotrophs	New Default	Old Default	Arrhenius
Max. spec. growth rate	3.200	3.200	1.029
Substrate half sat.	5.000	5.000	1.000
Anoxic growth factor	0.500	0.500	1.000
Aerobic decay	0.620	0.620	1.029
Anoxic/anaerobic decay	0.300	0.300	1.029
Hydrolysis rate (AS)	2.100	2.100	1.029
Hydrolysis half sat. (AS)	0.060	0.060	1.000
Anoxic hydrolysis factor	0.280	0.280	1.000
Anaerobic hydrolysis factor	0.500	0.500	1.000
Adsorption rate of colloids	0.800	0.800	1.029
Ammonification rate	0.040	0.040	1.029
Fermentation rate	3.200	3.200	1.029
Fermentation half sat.	5.000	5.000	1.000
Anaerobic growth factor (AS)	0.125	0.125	1.000
Hydrolysis rate (AD)	0.100*	5.000	1.050
Hydrolysis half sat. (AD)	0.150	0.150	1.000

*The default has changed in Version 2.1 because of a new kinetic formulation.

Methanol Utilizers	New Default	Old Default	Arrhenius
Max. spec. growth rate of methanol utilizers	6.400		1.029
Methanol half sat.	0.500		1.000
Aerobic decay rate of methanol utilizers	0.240		1.029
Anoxic/anaerobic decay rate of methanol utilizers	0.120		1.029

PolyP Heterotrophs	New Default	Old Default	Arrhenius
Max. spec. growth rate	0.950	0.950	1.000
Max. spec. growth rate, P-limited	0.420	0.420	1.000
Substrate half sat.	0.100	0.100	1.000
Substrate half sat., P-limited	0.050	0.050	1.000
Magnesium half sat.	0.100	0.100	1.000
Cation half sat.	0.100	0.100	1.000
Calcium half sat.	0.100	0.100	1.000
Aerobic decay rate	0.100	0.100	1.000
Anaerobic decay rate	0.040	0.040	1.000
Sequestration rate	6.000	6.000	1.000
Anoxic growth factor	0.330	0.330	1.000

Propionic Acetogens	New Default	Old Default	Arrhenius
Max. spec. growth rate	0.250	0.250	1.029
Substrate half sat.	10.000	10.000	1.000
Acetate inhibition	10000.0	10000.0	1.000
Decay rate	0.050	0.050	1.029
Aerobic decay rate	0.520	0.520	1.029

Methanogens	New Default	Old Default	Arrhenius
Acetoclastic Mu Max	0.300	0.650	1.029
H2-utilizing Mu Max	1.400	0.650	1.029
Acetoclastic Ks	100.0	200.0	1.000
H2-utilizing CO2 half sat.	0.100		1.000
H2-utilizing Ks	0.100	0.100	1.000
Acetoclastic propionic inhibition	10000.0	10000.0	1.000
Acetoclastic decay rate	0.130	0.130	1.029
Acetoclastic aerobic decay rate	0.600	0.600	1.029
H2-utilizing decay rate	0.130	0.130	1.029
H2-utilizing aerobic decay rate	0.600	0.600	1.029

4.2.2 SWITCHING FUNCTIONS

TABLE 4.3. SWITCHING FUNCTION PARAMETERS IN BioWin 2.

pH Inhibition Switches	New Default	Old Default
Heterotrophs low pH limit	4.00	
Heterotrophs high pH limit	10.00	
Methanol utilizers low pH limit	4.00	
Methanol utilizers high pH limit	10.00	
Autotrophs low pH limit	5.50	
Autotrophs high pH limit	9.50	
PolyP heterotrophs low pH limit	4.00	
Poly P heterotrophs high pH limit	10.00	
Heterotrophs low pH limit (anaerobic)	5.50	
Heterotrophs high pH limit (anaerobic)	8.50	
Propionic acetogens low pH limit	4.00	
Propionic acetogens high pH limit	10.00	
Acetoclastic methanogens low pH limit	5.50	
Acetoclastic methanogens high pH limit	8.50	
H2-utilizing methanogens low pH limit	5.50	
H2-utilizing methanogens high pH limit	8.50	

Switching Functions	New Default	Old Default
Heterotrophic DO limit	0.050	0.050
Aerobic denit. DO limit	0.050	0.050
Autotrophic DO limit	0.250	0.250
Anoxic NO3 limit	0.100	0.100
NH3 nutrient limit	0.005	0.005
NO3 nutrient limit	0.005	0.005

PolyP limit	0.010	0.010
VFA sequestration limit	5.000	5.000
P uptake limit	0.150	0.100
P nutrient limit	0.005	0.005
Heterotrophic Hydrogen limit	1.000	1.000
Propionic acetogens Hydrogen limit	5.000	5.000

4.2.3 STOICHIOMETRIC PARAMETERS

TABLE 4.4. STOICHIOMETRIC PARAMETERS IN BIOWIN 2.

Autotrophs	New Default	Old Default
Yield	0.240	0.150
N in biomass	0.070	0.068
N in inert	0.070	0.068
P in biomass	0.022	0.021
P in inert	0.022	0.021
Fraction to endogenous residue	0.080	0.080
COD:VSS ratio	1.420	1.420

Heterotrophs	New Default	Old Default
Yield (Aerobic)	0.666	0.666
Yield (fermentation low H2)	0.100	0.100
Yield (fermentation high H2)	0.100	0.100
Yield (fermentation of methanol)	0.100	0.100
H2 yield (fermentation low H2)	0.350	0.350
H2 yield (fermentation high H2)	0.0	0.0
H2 yield (methanol fermentation)	0.350	0.350
Propionate yield (fermentation low H2)	0.0	0.0
Propionate yield (fermentation high H2)	0.700	0.700
CO2 yield (fermentation low H2)	0.500	
CO2 yield (fermentation high H2)	0.0	
N in Biomass	0.070	0.068
N in Inert	0.070	0.068
P in Biomass	0.022	0.021
P in Inert	0.022	0.021
Endogenous Residue	0.080	0.080
COD:VSS Ratio	1.420	1.420
Yield (anoxic)	0.540	0.540
Yield propionic (Aerobic)	0.500	
Yield propionic (Anoxic)	0.410	
Yield acetic (Aerobic)	0.400	
Yield acetic (Anoxic)	0.320	
Yield methanol (Aerobic)	0.500	
Adsorp. max.	1.000	1.000

Methanol Utilizers	New Default	Old Default
Yield (anoxic)	0.400	
N in Biomass	0.070	
N in Inert	0.070	
P in Biomass	0.022	

P in Inert	0.022
Endogenous Residue	0.080
COD:VSS Ratio	1.420

PolyP Heterotrophs	New Default	Old Default
Yield (aerobic)	0.639	0.639
Yield (anoxic)	0.520	0.540
Aerobic P/PHA uptake	0.950	0.950
Anoxic P/PHA uptake	0.350	0.350
Yield of PHA on sequestration	0.889	0.889
N in biomass	0.070	0.070
N in part. inert	0.070	0.070
N in sol. inert	0.070	0.070
P in biomass	0.022	0.021
P in part. inert	0.022	0.021
Fraction to endogenous part.	0.250	0.250
Inert fraction of endogenous sol.	0.200	0.200
P/Ac release ratio	0.490	0.490
COD:VSS Ratio	1.420	1.420
Yield of low PP	0.940	0.940

Propionic Acetogens	New Default	Old Default
Yield	0.100	0.100
H2 yield	0.400	0.400
CO2 yield	1.000	
N in biomass	0.070	0.068
N in endogenous residue	0.070	0.068
P in biomass	0.022	0.021
P in endogenous residue	0.022	0.021
Fraction to endogenous residue	0.080	0.080
COD:VSS ratio	1.420	1.420

Methanogens	New Default	Old Default
Acetoclastic yield	0.100	0.100
H2-utilizing yield	0.100	0.100
N in acetoclastic biomass	0.070	0.068
N in H2-utilizing biomass	0.070	0.068
N in acetoclastic endog. residue	0.070	0.068
N in H2-utilizing endog. residue	0.070	0.068
P in acetoclastic biomass	0.022	0.021
P in H2-utilizing biomass	0.022	0.021
P in acetoclastic endog. residue	0.022	0.021
P in H2-utilizing endog. residue	0.022	0.021
Acetoclastic fraction to endog. residue	0.080	0.080
H2-utilizing fraction to endog. residue	0.080	0.080
Acetoclastic COD:VSS ratio	1.420	1.420
H2-utilizing COD:VSS ratio	1.420	1.420

4.2.4 GENERAL PARAMETERS

TABLE 4.5. GENERAL PARAMETERS IN BIOWIN 2.

General	New Default	Old Default
Particulate substrate COD:VSS ratio	1.600	1.600
Particulate inert COD:VSS ratio	1.600	1.600
Ash content of biomass (synthesis ISS) [%]	8.00	
Molecular weight of other anions [mg/mmol]	35.500	
Molecular weight of other cations [mg/mmol]	39.100	
Mg to P mole ratio in polyphosphate [mmol Mg/mmol P]	0.300	
Cation to P mole ratio in polyphosphate [meq/mmol P]	0.300	
Ca to P mole ratio in polyphosphate [mmol Ca/mmol P]	0.050	
Bubble rise velocity (anaerobic digester) [cm/s]	23.900	23.900
Bubble Sauter mean diameter (anaerobic digester) [cm]	0.350	0.350

Mass Transfer	New Default	Old Default
KI for H2 [m/d]	17.000	
KI for CO2 [m/d]	10.000	
KI for NH3 [m/d]	1.000	

4.2.5 PHYSICO-CHEMICAL PARAMETERS

TABLE 4.6. PHYSICO-CHEMICAL PARAMETERS IN BIOWIN 2.

Physico-chemical Rates	New Default	Old Default
Struvite precipitation rate [d]	3.00E+10	
Struvite redissolution rate [d]	3.00E+11	
Struvite half sat. [mg TSS/L]	1.000	
HDP precipitation rate [L/ (mol P d)]	1.00E+8	
HDP redissolution rate [L/ (mol P d)]	1.00E+8	
HAP precipitation rate [mol HDP/ (L d)]	5.00E-4	

Physico-chemical Constants	New Default	Old Default
Struvite solubility constant [mol/L]	6.918E-14	
HDP solubility product [mol/L]	2.750E-22	
HDP half sat. [mgTSS/L]	1.000	
Equilibrium soluble PO4 with Al dosing at pH 7 [mgP/L]	0.010	
Al to P ratio [mol Al/mol P]	0.800	
Al(OH)3 solubility product [mol/L]	1.259E+9	
AlHPO4+ dissociation constant [mol/L]	7.943E-13	
Equilibrium soluble PO4 with Fe dosing at pH 7 [mgP/L]	0.010	
Fe to P ratio [mol Fe/mol P]	1.600	
Fe(OH)3 solubility product [mol/L]	0.050	
FeH2PO4++ dissociation constant [mol/L]	5.012E-22	

4.2.6 AERATION PARAMETERS

TABLE 4.7. AERATION PARAMETERS IN BioWin 2.

Aeration Parameters	New Default	Old Default
Alpha (surf) OR Alpha F (diff) []	0.500	0.500
Beta []	0.950	0.950
Surface pressure [kPa]	101.325	101.325
Fractional effective saturation depth (Fed)	0.325	0.325
Supply gas CO2 vol. %	0.035	
Supply gas O2 vol. %	20.950	
Off-gas CO2 vol. %	2.000	
Off-gas O2 vol. %	18.800	
Off-gas H2 vol. %	0.0	
Off-gas NH3 vol. %	0.0	
Surface turbulence factor	0.250	
Set point controller gain []	1.000	1.000

4.2.7 SETTLING PARAMETERS

TABLE 4.8. SETTLING PARAMETERS IN BioWin 2.

Modified Vesilind Settling Parameters	New Default	Old Default
Maximum Vesilind settling velocity (Vo) [ft/min]	0.3873	0.3873
Vesilind hindered zone settling parameter (K) [L/g]	0.370	0.370
Clarification switching function [mg/L]	100.0	20.0
Specified TSS conc. for height calc. [mg/L]	2500.0	2500.0
Maximum compactability constant [mg/L]	15000.0	15000.0

Double Exponential Settling Parameters	New Default	Old Default
Maximum Vesilind settling velocity (Vo) [ft/min]	0.9341	
Maximum (practical) settling velocity (Vo') [ft/min]	0.6152	
Hindered zone settling parameter (Kh) [L/g]	0.4000	
Flocculent zone settling parameter (Kf) [L/g]	2.500	
Maximum non-settleable TSS [mg/L]	20.0	
Non-settleable fraction []	0.001	
Specified TSS conc. for height calc. [mg/L]	2500.0	

4.2.8 MISCELLANEOUS

TABLE 4.9. MISCELLANEOUS PARAMETERS IN BioWin 2.

Parameter	New Default	Old Default
Influent ISS [mg/L]	45	15
Influent F_{NA} – ammonia/TKN	0.66	0.75
Influent $F_{UP,N}$	0.035	0.068
Influent $F_{UP,P}$	0.011	0.022
Ideal clarifier solids removal [%]	99.8	99.99