EnviroSim ASSOCIATES LTD.

PetWin

New Developments in PetWin 4.1

PetWin 4.1 continues to expand the capabilities of wastewater treatment plant simulation with key enhancements to the core model, the model library, and the interface. A focus in this release has been to extend and refine the core Industrial Activated Sludge Digestion Model (ASDMi) model, which builds on the industry-standard BioWin model to include over 100 processes acting on over 60 state variables related to industrial wastewater compounds. In addition to adding many new process rate equations, refinements to the core model have resulted in faster dynamic simulations, particularly for nutrient removal systems.

New Models and Processes

The most significant ASDMi extension has been to include three mechanisms for modeling nitrous oxide (N_2O) production and emission. As a result, PetWin 4.1 is a powerful tool for evaluating plant-wide greenhouse gas (GHG) emissions of nitrous oxide, methane and CO_2. The basis of the N_2O model, and other extensions and improvements to the ASDMi are outlined further below.

New flowsheet elements for trickling filters, thermal hydrolysis (sludge digestion pre-treatment), submerged aerated filters, and sidestream media bioreactors have been added for increased modeling flexibility. Enhancements have been made for several existing flowsheet elements including primary settling tanks, cyclones, and anaerobic digesters.

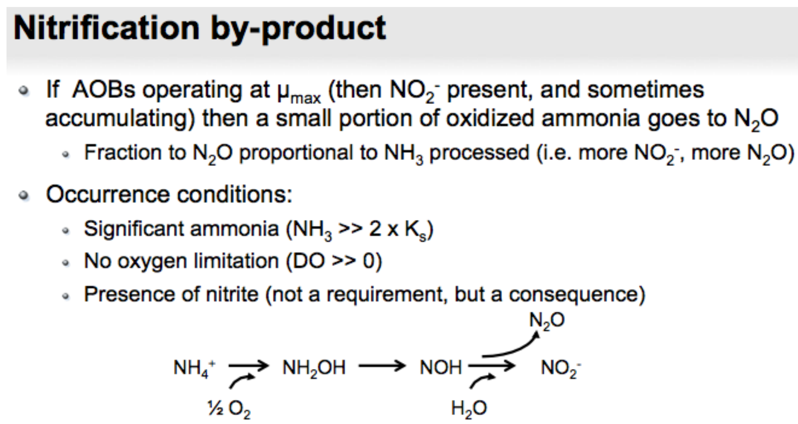
1.0 ASDMi Model Additions and Updates

1.1 New Model – Nitrous Oxide Emission

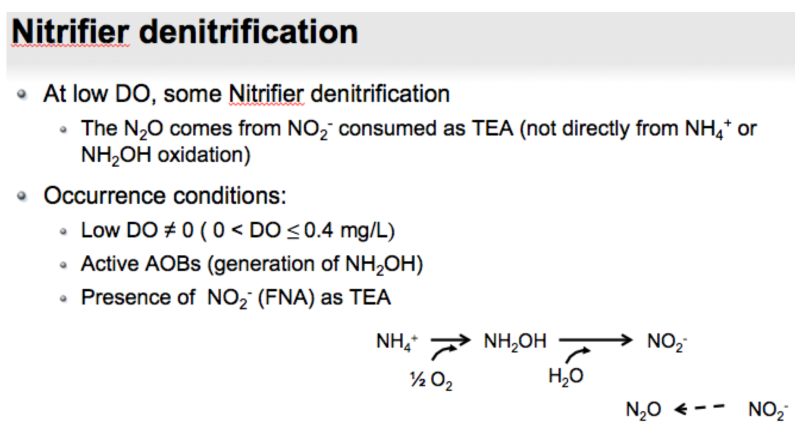
Nitrous oxide has a global warming potential 300 times higher than carbon dioxide and can be a significant source of greenhouse gas (GHG) emissions from wastewater treatment plants. EnviroSim conducted an extensive multi-year study on the GHG issue of nitrous oxide production and emission from activated sludge processes. A comprehensive review of published literature was conducted, assembling state of the art knowledge and resolving incompatibilities amongst the various approaches. Much experimental work was performed to substantiate our understanding and support the development of nitrous oxide models in the PetWin ASDMi model.

The outcome of these efforts is embodied in the ASDMi model as three major process mechanisms for potential nitrous oxide production. Two of these are mediated by ammonia oxidizing biomass (AOBs) and one by heterotrophs in denitrification, as described below.

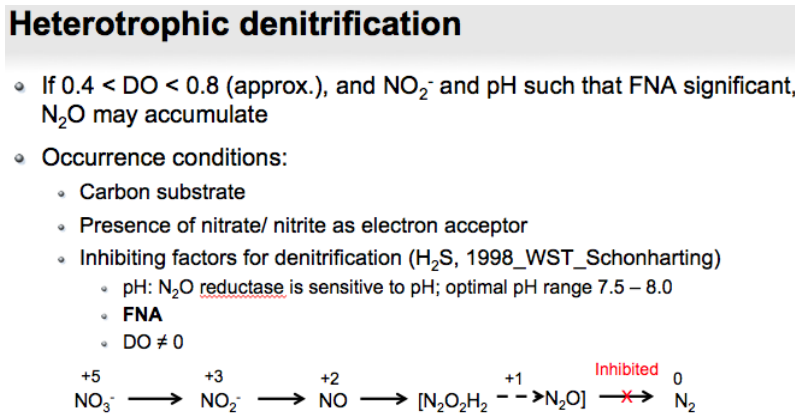
1. **Nitrification byproduct:** When AOBs are operating at maximum rate in the presence of ammonia excess, and with no oxygen limitation, a small fraction of the oxidized ammonia is directed to N_2O.



2. **Nitrifier denitrification by AOBs:** Under oxygen-limited conditions where nitrite is present, free nitrous acid (FNA) can be used as a terminal electron acceptor, and is converted to N_2O.

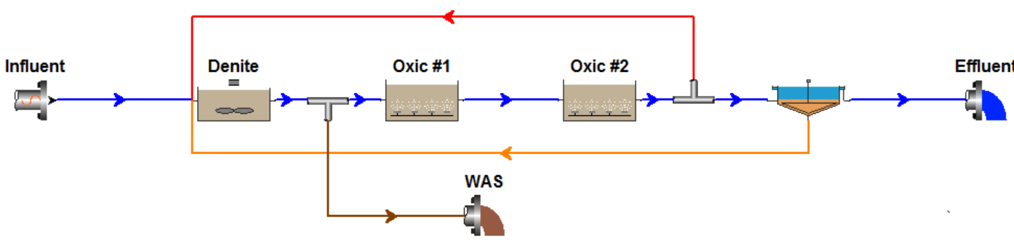


3. **Heterotrophic denitrification:** At low DO, and depending on nitrite concentration and pH, free nitrous acid (FNA) reaches a level where the final step of denitrification is inhibited, and N_2O accumulates.



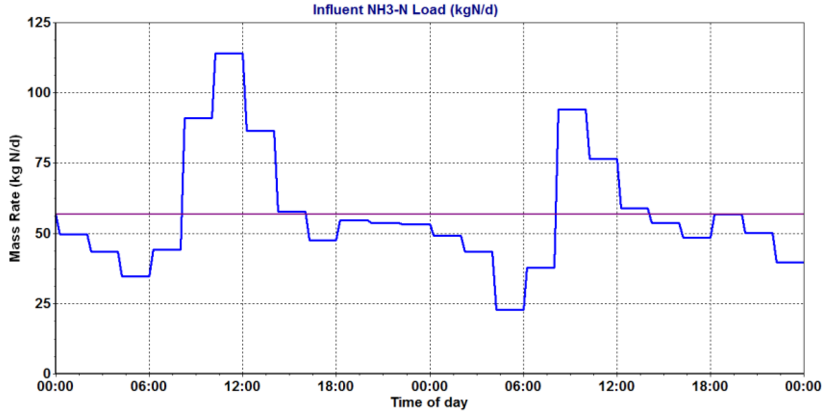
1.1.1 PetWin 4.1 Nitrous Oxide Model Example

The following example illustrates PetWin 4.1 nitrous oxide modeling capabilities using data from a pilot plant operated by the Swiss Federal Institute of Aquatic Science and Technology (EAWAG). Mixed liquor is recycled from the aerobic zone to an anoxic zone for denitrification at a ratio of 150% of the influent flow. The clarifier underflow is recycled to the anoxic reactor at a ratio of 250% of the influent flow. The SRT is maintained at 12.5 days.

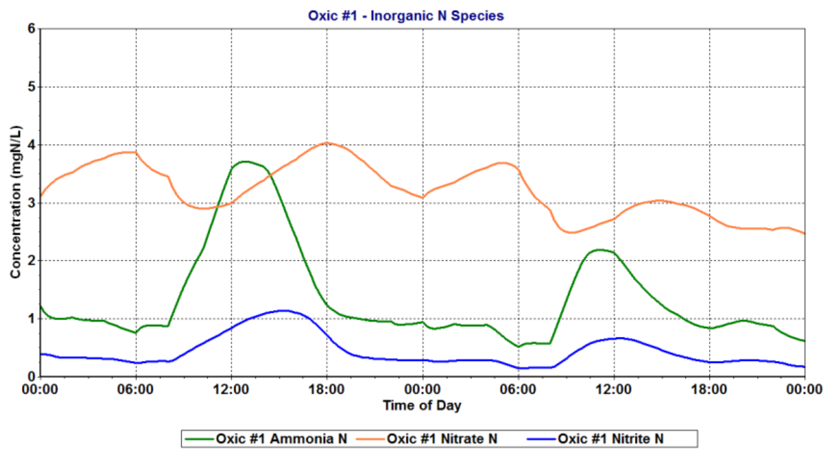


Pilot Plant Process Diagram

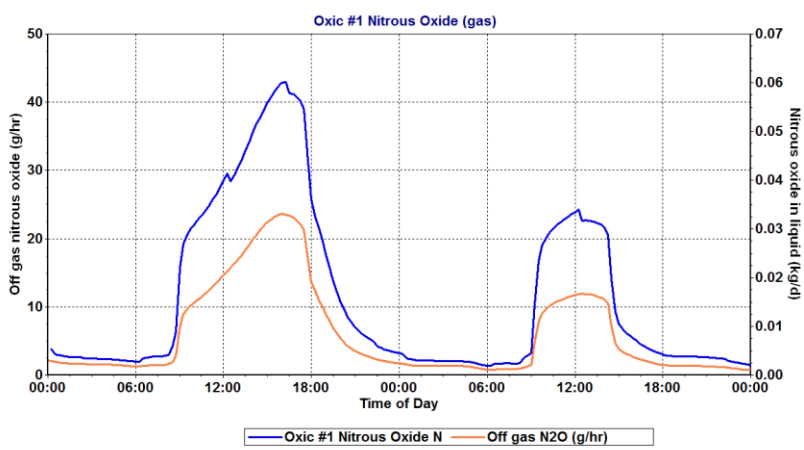
The following three plots show the varying influent ammonia-N load over two days, the varying nitrogen species concentrations (ammonia, nitrate, and nitrite) in the first aerated bioreactor [Oxic #1], as well as the mass rate of nitrous oxide in the off-gas and the liquid output from Oxic #1. The ammonia concentration in Oxic #1 increases above 2 mgN/L when the influent ammonia load peaks. Simultaneously the nitrous oxide emissions elevate in the presence of excess ammonia (Mechanism #1).



Ammonia-N influent loading



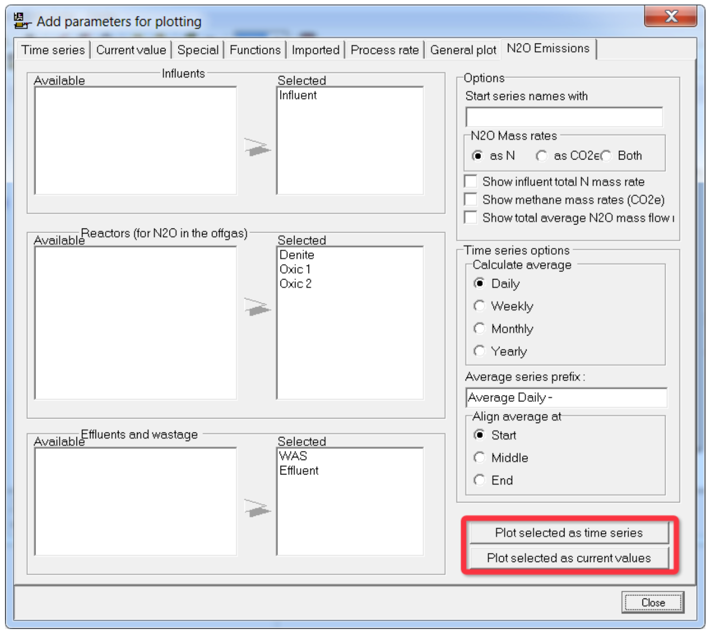
Nitrogen species in aerated bioreactor Oxic #1



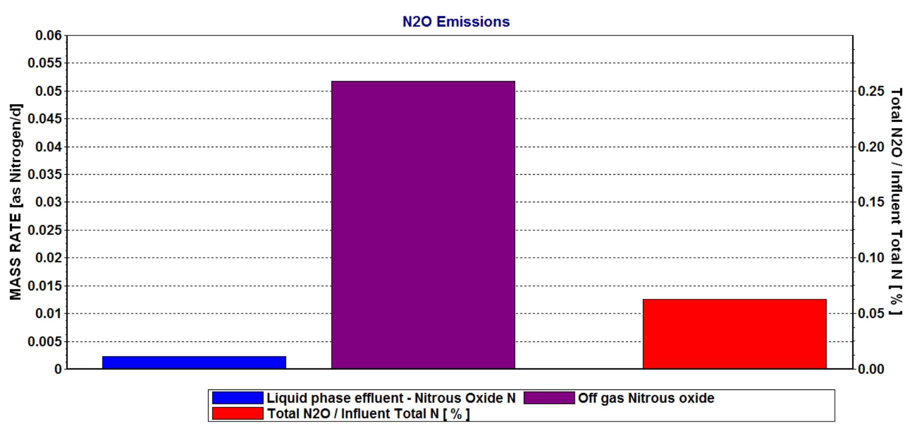
Nitrous Oxide from aerated bioreactor Oxic #1

PetWin 4.1 provides the means for rapidly generating a plant-wide plot of nitrous oxide emissions. To set up the N_2O emissions chart:

- Influent elements are selected to calculate the total nitrogen input load;
- Reactors are selected to estimate off-gas N_2O emission;
- Waste/ effluent streams are selected to estimate N_2O in the liquid stream outputs.

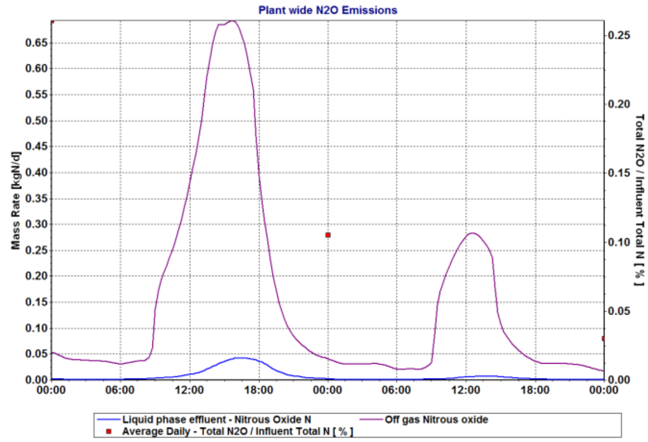


A current value plot typically is selected to demonstrate steady state estimation results. The mass rate of N_2O in the outflows and the total mass rate of N_2O leaving the system via gas and liquid are plotted against the left axis in units of kgN/day (or lbN/day), while the N_2O emission via off-gas as a percentage of the total influent nitrogen load is plotted to the right axis.



Steady-State Plant-wide Nitrous Oxide Emissions

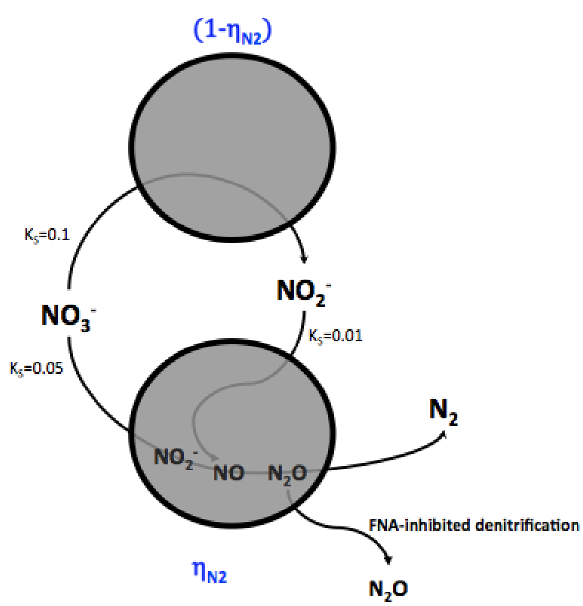
A time series chart should be selected to demonstrate dynamic estimation results. In addition to the mass rate of N_2O in the effluent, total mass rate of N_2O in the off-gas and liquid, and the percentage of N_2O in off-gas out of influent nitrogen, the daily average percentage N_2O emission in off-gas is also plotted.



Dynamic Plant-wide Nitrous Oxide Emissions

1.2 Model Update – Denitrification

EnviroSim's ongoing model development and in-house experimental work has led to the adoption of a novel denitrification model structure. In PetWin 4.1, denitrification follows two pathways within the heterotroph population. One fraction of the population reduces nitrate only as far as nitrite. The remaining population fraction reduces both nitrate and nitrite to nitrogen gas (without releasing intermediates under normal circumstances). Where nitrite is present in the liquid, and free nitrous acid (FNA) concentration is significant (also depends on pH), this population fraction can reduce NOx to dissolved N_2O rather than nitrogen gas.



PetWin Denitrification Model

In PetWin 3.1, denitrification is modeled as a two-step series process. That is, nitrate is reduced to nitrite (and the nitrite implicitly is excreted to the liquid phase), and then nitrite is taken up and converted to nitrogen gas, without tracking intermediates. In recent modeling literature, particularly where nitrous oxide is a concern, a 4-step denitrification path (nitrate - nitrite - nitric oxide - nitrous oxide - nitrogen gas) is often adopted. In these approaches, it is implied that each intermediate is expressed into the liquid phase and immediately taken up again for the subsequent step; seemingly impractical from an energetic point of view.

The PetWin 4.1 model was implemented after extensive investigation and research which included a comprehensive literature review and experimental work. Experiments conducted in support of denitrification model refinement included unaerated batch tests combining mixed liquor and municipal wastewater for the evaluation of issues such as (a) nitrate *versus* nitrite removal rates when batch tests are spiked with each electron acceptor separately; (b) nitrite accumulation; and (c) removal rates when both nitrate and nitrite are available in similar concentrations.

As a result of this effort, the PetWin 4.1 denitrification model now allows for tracking of key intermediates such as nitrous oxide, and a robust mathematical approach which better approximates the denitrification process. Note that these denitrification model changes also impact anoxic processes involving industrial components. Further details can be found in the PetWin User Manual.

1.3 Model Addition – Decay of Endogenous Residue

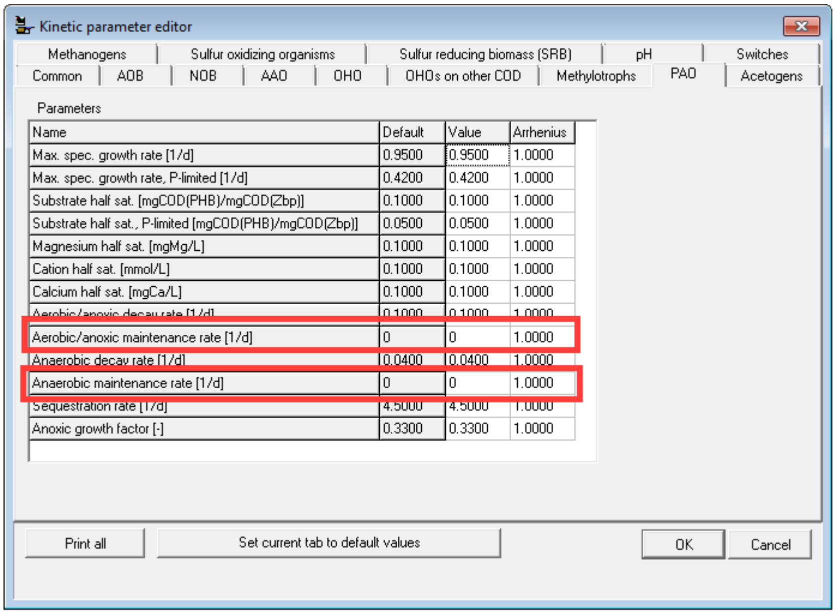
PetWin allows for the conversion of endogenous decay products to biodegradable particulate substrate. This is modeled as a first order process with respect to the concentration of the endogenous products. Nitrogen and phosphorus included in the endogenous matter are lyzed in parallel as particulate organic N and P.The default process rate constant is set at zero. The user should specify a small value (e.g. 0.007 /day) to simulate this slow decay process.

1.4 Model Extension – PAO Lysis Decay *versus* Maintenance Approach

Several studies of biological phosphorus removal in EBPR systems in recent years have focused on systems implementing non-conventional methods such as fermentation of return activated sludge (RAS) or mixed liquor solids (MLSS) as a means for improving EBPR performance. Regarding modeling of EBPR in these non-conventional systems, it has been suggested that the method for modeling PAO biomass decay may be an important factor in correctly predicting EBPR performance [*e.g.* Houweling *et al*., 2010]. Specifically it has been suggested that the maintenance approach proposed by the Technical University of Delft (TUD) may offer some advantages over the University of Cape Town decay/lysis approach applied in PetWin.

The ability to choose the Delft approach in place of the PetWin approach has been included in PetWin 4.1. Rate parameters for the maintenance approach are assigned values of zero. The user should assign appropriate values (and set PAO aerobic/anoxic and anaerobic decay rates to zero) to apply the Delft approach if desired.

It is worth noting that both decay approaches have been evaluated recently as part of a WERF study. The general finding was that either approach has little impact on EBPR performance predictions. This likely is due to the slow decay rates of PAOs, and that decay has a limited impact on model predictions compared to other model processes.



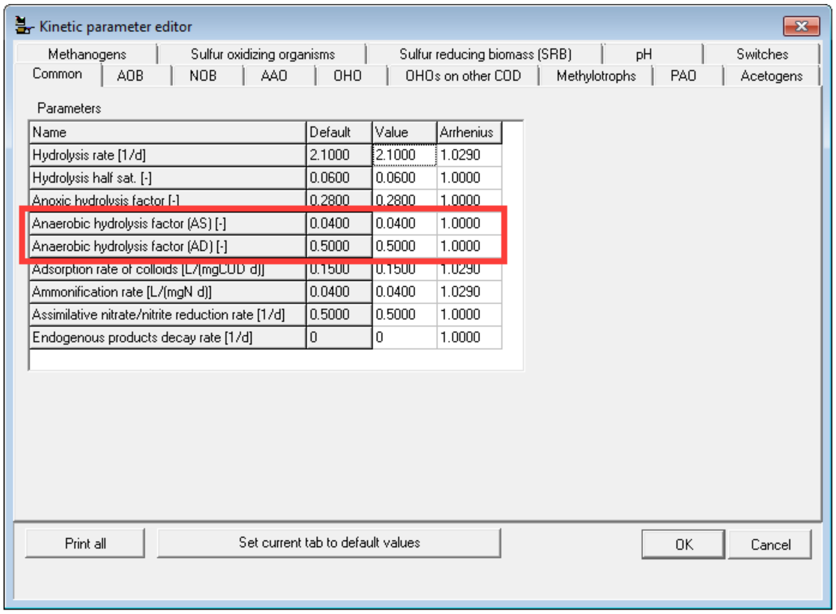
Delft Maintenance Approach Parameters

1.5 Model Update – Unified Hydrolysis Formulation

Different kinetic expressions were employed in PetWin 3.1 for the hydrolysis of particulate organic substrate mediated by activated sludge and anaerobic digestion. In Version 4.1, the kinetic expression for activated sludge hydrolysis is now also applied in anaerobic digesters. However, based on calibration, the *Anaerobic hydrolysis factor [AD]* applied in anaerobic digesters and active primary settlers is higher than the *Anaerobic hydrolysis factor [AS]* applied in anaerobic zones of activated sludge bioreactors.

The activated sludge anaerobic factor is lower than the default in PetWin 3.1; that value appeared to result in excessive VFA generation as a result of too much hydrolysis.

The unified hydrolysis formulation allows PetWin 4.1 users to effectively use an activated sludge element to model a non-conventional fermenter (such as a RAS fermenter) and obtain similar results as with an anaerobic digester element.



Anaerobic Hydrolysis Factor Defaults

1.6 Model Changes – Parameter Default Changes

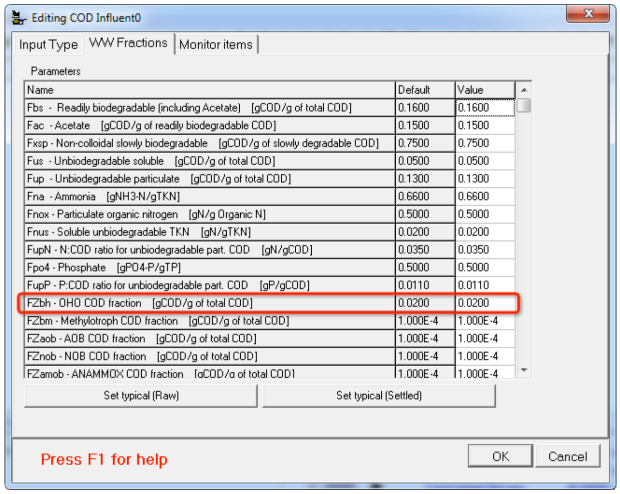
A few parameter default values in PetWin are changed in Version 4.1. Mostly these are very minor changes. However, attention should be drawn to two specific changes:

- Heterotroph biomass COD fraction in Influent elements;
- Bio-P model parameters (four values adjusted).

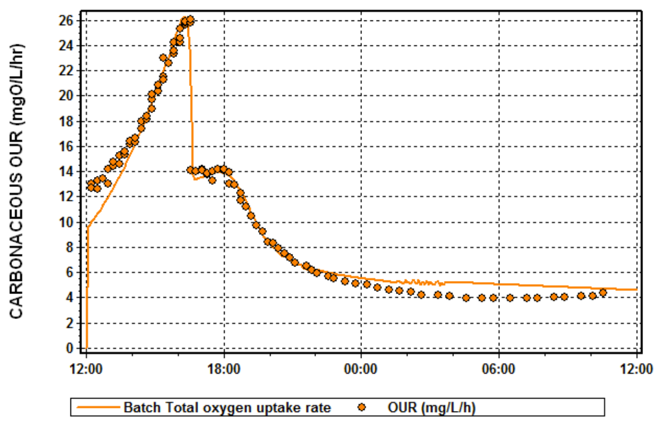
1.6.1 Influent Biomass

Traditionally it has been assumed that municipal influent wastewater contains a minimal amount of active biomass. Over the past three years EnviroSim has conducted extensive testing on influent wastewaters from many plants to quantify the heterotrophic biomass content. The Wentzel/UCT batch method has been applied where the oxygen utilization rate in a non-seeded influent wastewater sample is expected to increase exponentially over the first part of the test, starting from an initial low value (e.g. 1-2 mg/L/hour). Many of the EnviroSim experiments have indicated the active biomass content in the influent wastewater is appreciable. The plot below shows an example OUR response. The initial high OUR and the near-linear increase in OUR both indicate an appreciable amount of active heterotrophs in the wastewater.

The COD and BOD Influent element default COD fractions of heterotrophs (f_{Zbh}) in PetWin 4.1 are changed to 0.02 to replace the previous value of 0.0001.



New default f_{Zbh} (COD fraction of heterotrophs in influent) of 0.02



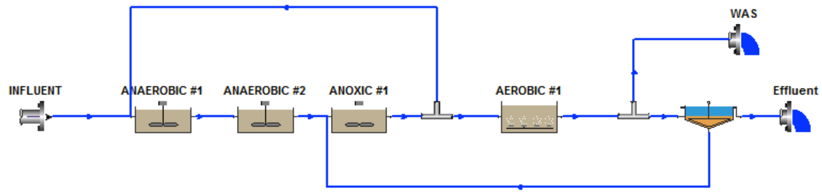
Example OUR response with default f_{Zbh} = 0.02

1.6.2 Refined Bio-P Model Parameters

EnviroSim has conducted a thorough review of the biological P removal model predictions in light of other model changes such as the unified hydrolysis expression. The review was conducted by evaluating predictions of performance for many pilot-scale systems. As a result, default values for a few parameters have been adjusted slightly. The refined parameters include:

- Cation uptake
- Sequestration rate
- Aerobic P/ PHA ratio
- P/ Ac ratio

The predictive capacity of the model is demonstrated below for one of the pilot enhanced biological phosphorus removal (EBPR) systems (Wentzel's System 8a). This was a UCT configuration with recycle ratios of nitrified mixed liquor and clarifier underflow both at 100% of the influent flow. The SRT of the system was about 9 days.



The plots below show predictions for a range of parameters: VSS, OUR, phosphate and nitrate concentration profiles, and effluent TKN and COD. Good predictions of plant performance are achieved with the refined model parameters.

1.6.3 Refined Biofilm Model Parameters

For biofilms, the default EPS factors for nitrifiers (AOBs and NOBs) have been increased. This change was based on extensive assessment of nitrification performance in IFAS systems.

1.7 Minor Model Refinements

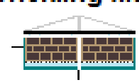
The following minor changes are worth noting:

- Stoichiometry to allow specifying different N and P contents in each biomass and in endogenous residue;

- Gas phase modeling has been rationalized, and all gases now use the same form of Henry's Law expression to determine saturation concentrations. These are editable, and the user can specify temperature dependency;
- For bioreactors, upper and lower airflow limits can be set and also manipulated from BW Controller;
- SRT calculations can include or exclude biofilm mass for attached growth systems.

2.0 New Elements & Element Enhancements

2.1 New Element – Trickling Filter



A new process flowsheet element has been added for Trickling Filters. The Trickling Filter (TF) unit can be configured for various default packing types (e.g. rock or plastic media), or the user can customize packing characteristics. The flowsheet image for the trickling filter changes depending on the type of media selected.

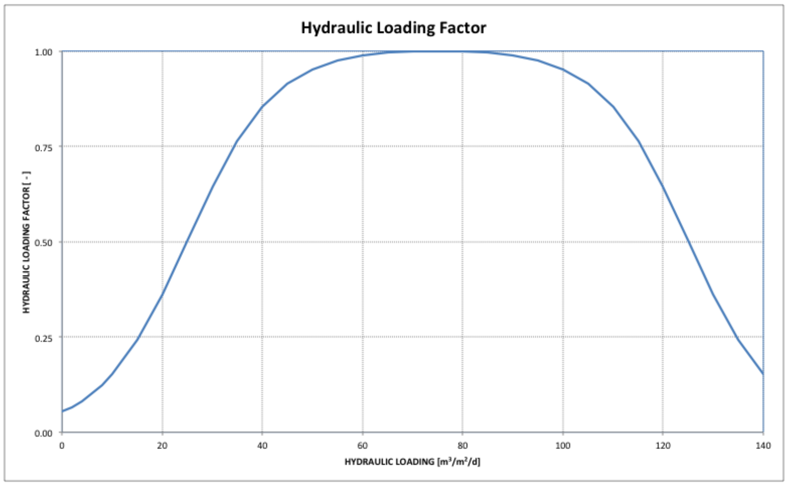
The depth of the trickling filter is divided into three sections or 'slices' of equal height with liquid distributed evenly over the top surface. The sections are used for modeling aspects such as oxygen transfer from the top of the trickling filter to the bottom (if the gas phase modeling feature of PetWin is used) and also to simulate removal gradients down the depth of the trickling filter.

On the *Media and model specification* tab the user specifies the type of trickling filter media to be used. Note that trickling filter elements in PetWin are assumed to be 100% full of media. The following media choices are available: Rock, Horizontal, Structured plastic (crossflow), Loose media (random), and Custom. Toggling between the first four of these changes the specific area and specific volume (i.e. 1-porosity) fields to commonly accepted values for those parameters. For custom media, the specific area and specific volume can be adjusted. Users also specify the number of layers to use for modeling the biofilm attached to the media and the liquid boundary layer thickness.

The total thickness of the liquid layer covering the biofilm can be specified for any type of media. This is used to calculate the hydraulic residence time of the trickling filter. Making this parameter larger will increase the hydraulic residence time, and making it smaller will decrease the hydraulic residence time (all other things being equal). Performance of the trickling filter is related to hydraulic loading by making the area available for gas transfer to the liquid phase dependent on the liquid velocity through the trickling filter (thereby making more or less oxygen available to the biofilm).

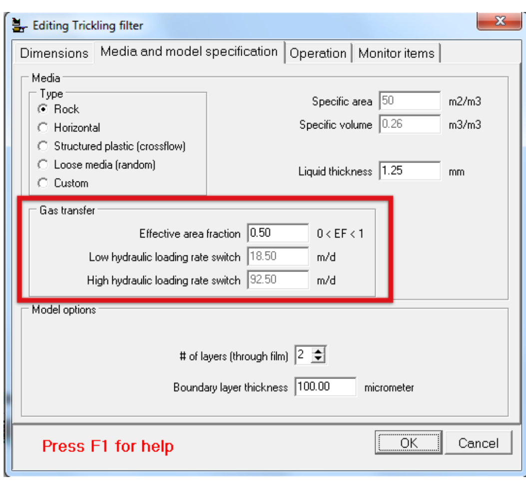
Oxygen transfer is a most important factor in determining trickling filter behaviour. The user has considerable flexibility to manipulate aeration through specifying DO concentrations or air flow rates, and selecting whether to model gas phase composition. DO concentrations in the liquid phase can be specified as uniform for each section, or PetWin can model the profile through the filter.

Hydraulic loading rate may impact the area available for gas transfer in PetWin. If the hydraulic loading rate is too low then not all of the media will be "wet" so the gas transfer area will be reduced. On the other hand, if the hydraulic loading rate gets too high then it is possible that the air spaces between the media will be flooded, which also will reduce the available gas transfer area. The **Hydraulic Loading Factor** attempts to account for these less-than-optimal conditions. The **Hydraulic Loading Factor** is determined by a two-sided continuous switching function; an example is shown below:

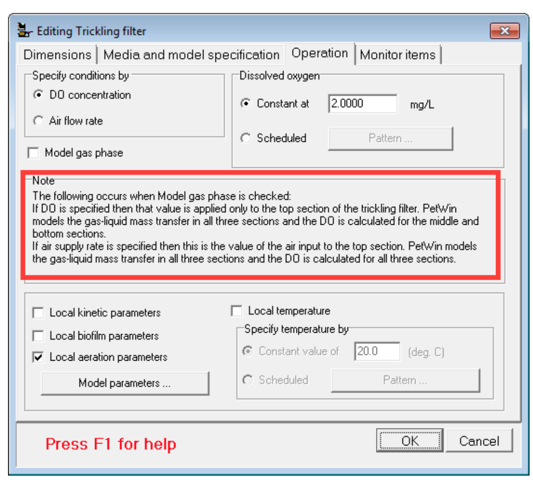


Hydraulic loading factor as a function of hydraulic loading

Over an optimal range of hydraulic loading rates the **Hydraulic Loading Factor** is equal to or close to unity (1). The value decreases towards zero for extreme low or high loading rates. The form of the continuous switching function is defined by the **Low hydraulic loading rate switch** value and the **High hydraulic loading rate switch** value. These are the low and high hydraulic loading rates where the **Hydraulic Loading Factor** has a value of 0.5 (*i.e.* the area for gas transfer is reduced to half of the effective area). Different media types have characteristic high and low loading rates. These are shown in the **Low hydraulic loading rate switch** and **High hydraulic loading rate switch** fields (highlighted in the picture below), and these change accordingly when any of the first four media types are selected. If **Custom** is selected, the user may edit the switch values on the *Media and Model Specification* tab.

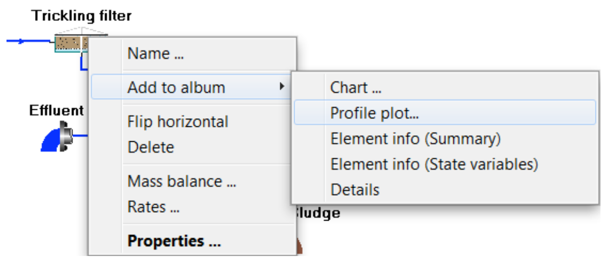


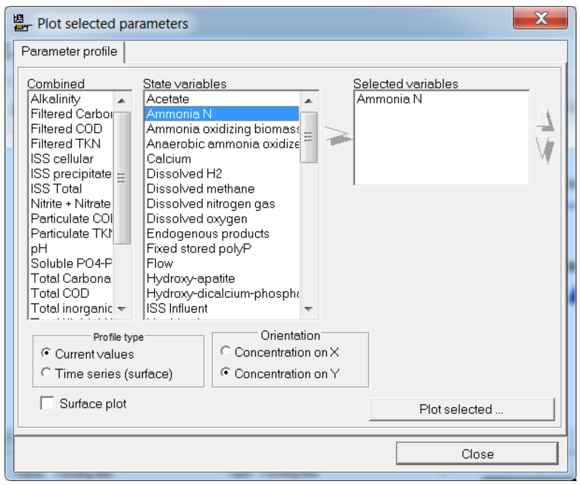
Trickling Filter – Media and Model Specification

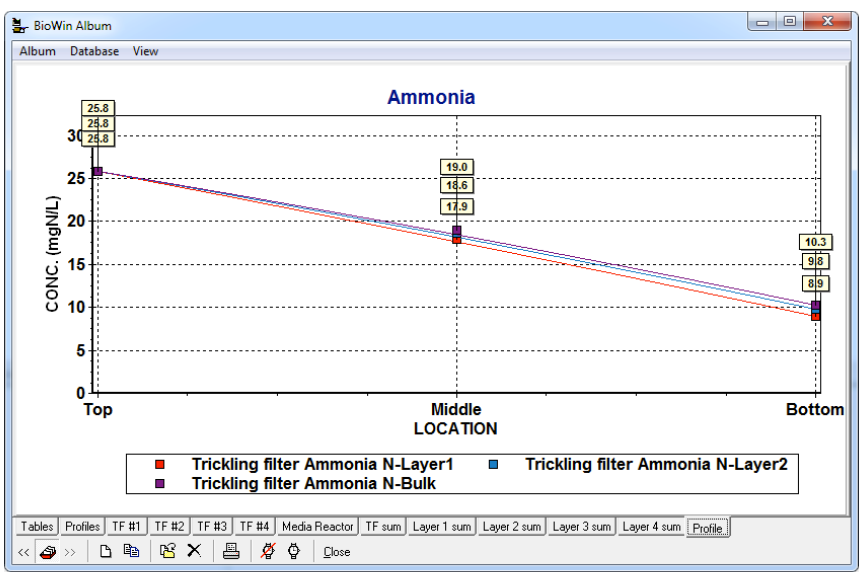


Trickling Filter – Operating Parameters

Profiles can be plotted to show concentration gradients through the depth of the trickling filter (top, middle, and bottom ‘slice’) as well as the concentrations in each biofilm layer and in the bulk liquid within each ‘slice’ of filter.



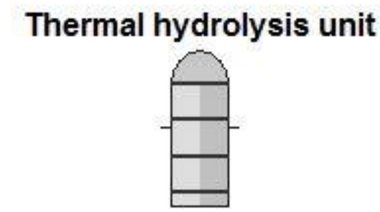


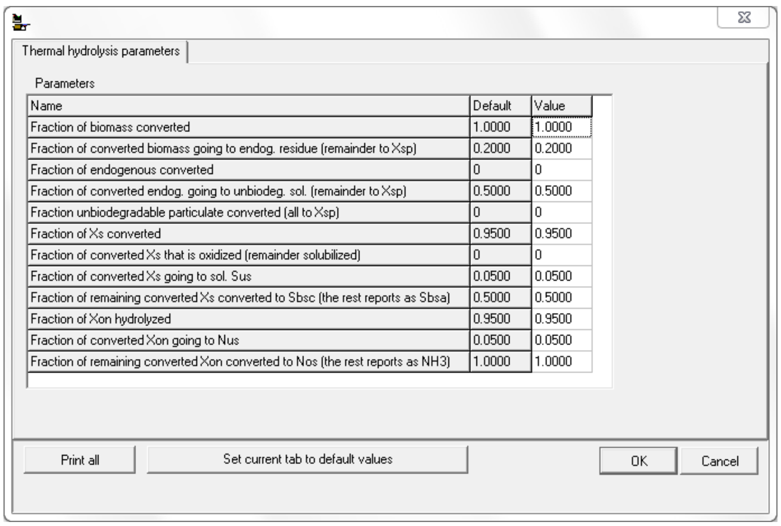


Trickling Filter Ammonia-N Concentration Profile

2.2 New Element – Thermal Hydrolysis Unit

A Thermal Hydrolysis (TH) element has been added to simulate the breakdown of particulate components in a sludge stream generally into various soluble components. The TH unit is a dimensionless mass balance converter that instantaneously converts the particulate state variables into predefined sets of other state variables, and the user defines the extent of conversion and the fractional distribution between ‘products’ of hydrolysis. This highly flexible flowsheet element allows PetWin users to simulate a variety of sludge pretreatment technologies such as ozonation, sonication and chemical oxidation.




Thermal hydrolysis parameters

Parameters

Name	Default	Value
Fraction of biomass converted	1.0000	1.0000
Fraction of converted biomass going to endog. residue (remainder to Xsp)	0.2000	0.2000
Fraction of endogenous converted	0	0
Fraction of converted endog. going to unbiodeg. sol. (remainder to Xsp)	0.5000	0.5000
Fraction unbiodegradable particulate converted (all to Xsp)	0	0
Fraction of Xs converted	0.9500	0.9500
Fraction of converted Xs that is oxidized (remainder solubilized)	0	0
Fraction of converted Xs going to sol. Sus	0.0500	0.0500
Fraction of remaining converted Xs converted to Sbsc (the rest reports as Sbsa)	0.5000	0.5000
Fraction of Xon hydrolyzed	0.9500	0.9500
Fraction of converted Xon going to Nus	0.0500	0.0500
Fraction of remaining converted Xon converted to Nos (the rest reports as NH3)	1.0000	1.0000

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The TH unit parameter editor allows users to specify the degree to which major particulate components of sludge VSS (biomass [Z], endogenous residue [Z_E], unbiodegradable particulate COD [X_I], biodegradable particulate COD [X_{SP}]) will be affected by the thermal hydrolysis process. The user may also specify the fraction of biodegradable particulate organic nitrogen [X_{ON}] that is hydrolyzed by pretreatment.

The default conversion fractions in the thermal hydrolysis unit were derived empirically to reflect the conversions typically observed when WAS is treated in a batch high-pressure thermal hydrolysis (HPTH) process at 160 to 170°C at 7 bars for approximately 30 minutes. The performance indicators associated with this pretreatment are summarized in the following table:

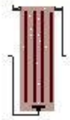
ATTRIBUTE	VALUE
VSS Destruction	30 to 50 %
COD Solubilization	30 to 50 %
Inert Soluble COD Generation	2 to 5 %
Organic N Solubilization	30 to 50 %
TCOD	Conserved
TN	Conserved
Biomass	Inactivated

Note: BioWin Advantage Volume 3 (Number 2) [downloadable from www.envirosim.com] illustrates application of the thermal hydrolysis unit.

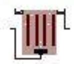
2.3 New Element – Submerged Aerated Filter

A submerged aerated filter (SAF) element has been added to simulate bioreactors with fully submerged fixed media in an upflow configuration. There are two types of SAFs available: 1) a standard SAF in which the depth is divided into three "slices" and there is a liquid volume and a biofilm mass/volume associated with each "slice"; and 2) a "shallow" SAF which has one completely mixed liquid volume and one biofilm mass/volume for the whole unit. As a result, the "shallow" SAF is less plug-flow in nature than the standard SAF.

Submerged aerated filter



Shallow submerged aerated filter



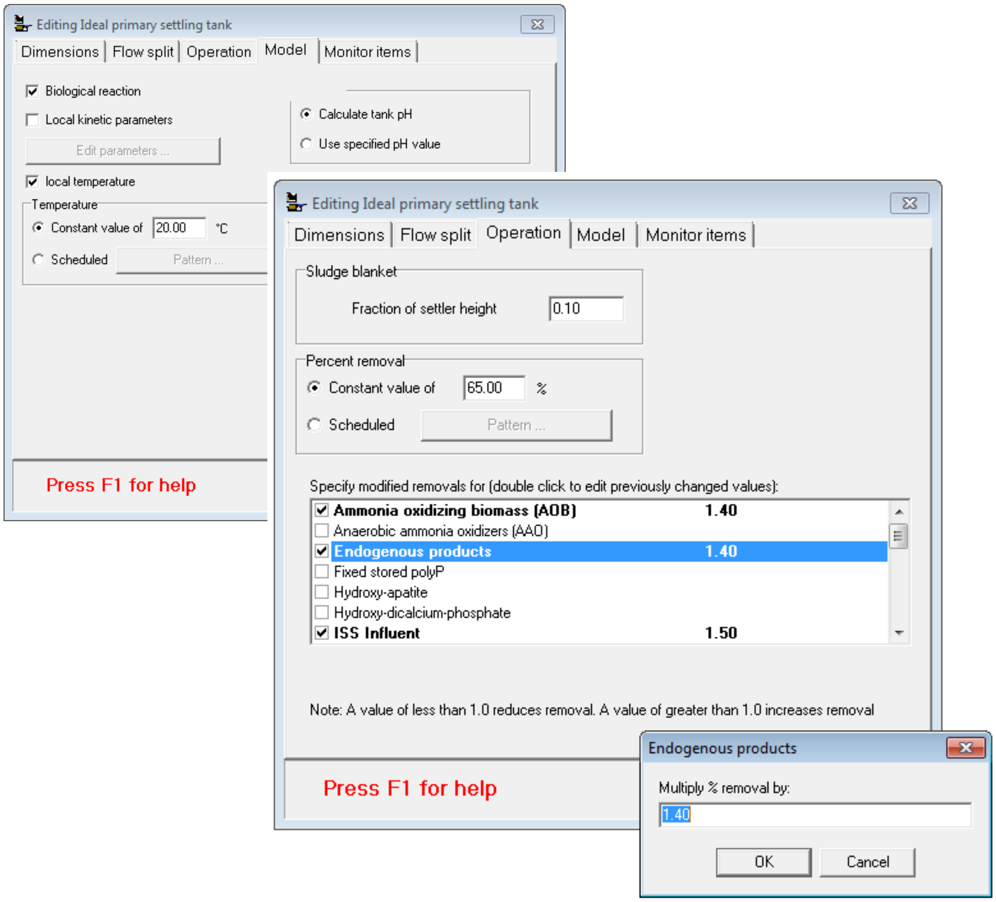
2.4 New Element – Sidestream Media Bioreactor

Side stream media bioreactor

Media bioreactors using IFAS or MBBR biofilm-based systems are being applied more widely in the context of sidestream treatment; for example, for deammonification of digester centrate streams. The existing Media Bioreactor in PetWin can be used for these systems. However, for convenience a Side Stream Media bioreactor has been added. The only difference from the existing Media Bioreactor is that this new unit is seeded with different initial concentrations more appropriate for sidestream conditions. Also, the default temperature is set to 35°C.

2.5 Element Enhancement – Ideal Primary Settling Tank

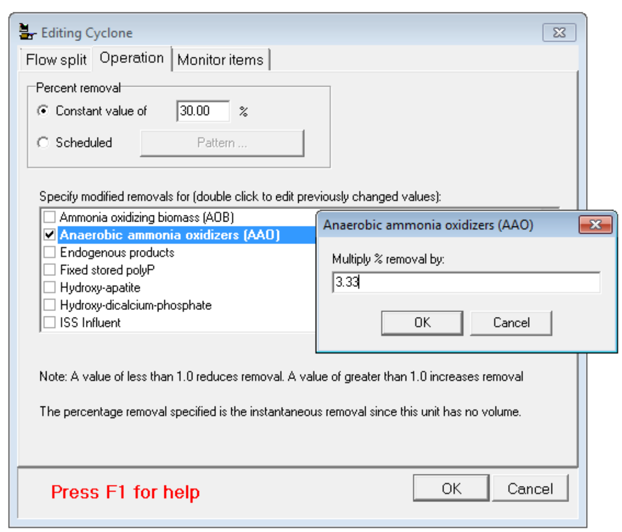
- The Ideal Primary Settling Tank element now has a Model tab which allows biological reactions to be toggled on or off. With this addition, the Activated Primary Settling tank is redundant. Existing flowsheets from earlier PetWin versions containing Activated Primary Settling Tank elements will be automatically converted to the new Ideal Primary Settling Tank elements with no change in functionality.
- It is now possible to specify individual removal percentages for particulate state variables across a primary settling tank element. For example, users can specify additional removal of inert suspended solids to simulate a changing VSS/TSS ratio across a primary settling tank.
- Percentage removals for TKN, TP, COD, BOD, and TSS are now calculated automatically and can be displayed in Album tables or charts.
- When pointing at a primary settling tank element on the flowsheet, the summary view in the main PetWin window now displays Percent TSS, COD, and BOD removal.



2.6 Element Enhancement – Cyclones

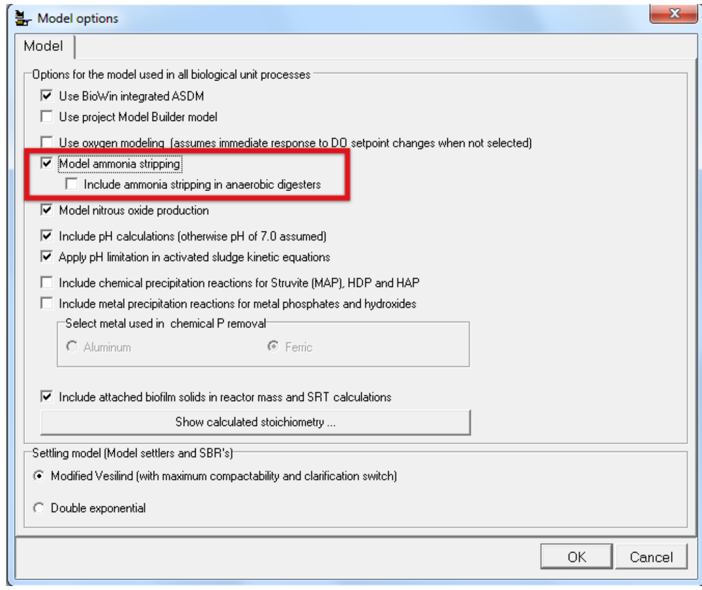
The Cyclone element now allows for individual removal percentages for particulate state variables. This is useful for simulating cyclones and other solids separation technologies proposed for certain mainstream deammonification processes. These rely on preferential retention of anaerobic ammonia oxidizing organisms.

PetWin also includes an ISS Cyclone that preferentially captures only influent inorganic suspended solids.



2.7 Element Enhancement – Anaerobic Digester

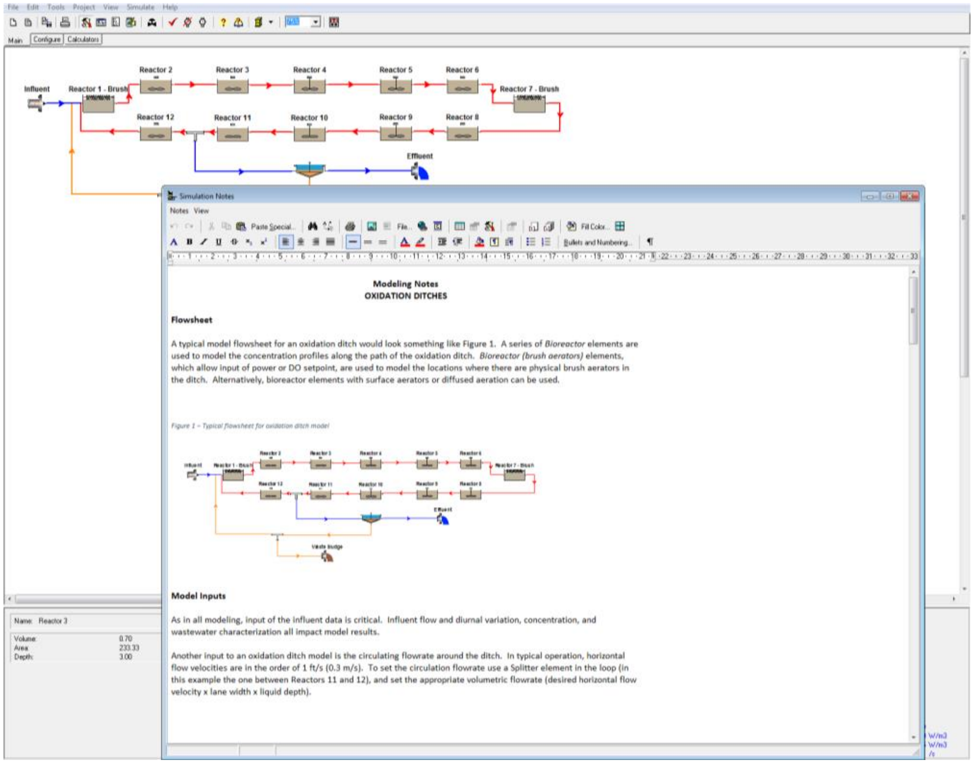
Ammonia stripping in anaerobic digesters is now a model option that can be toggled on or off. Simulation speeds can be increased if ammonia stripping is not needed in the model.



3.0 Usability Improvements

PetWin 4.1 usability improvements include:

- PetWin's Notes Editor has gained significant functionality and now has full Rich Text Format (RTF) capability. Project notes can now contain tables, screenshots from the PetWin Album, and other useful formatting components. The notes also can be easily exported to Word, to streamline your project reporting workflow.



- Any notes added with PetWin's internal Notes Editor are now saved internally to the PetWin file (as opposed to a separate "*.nts" file in previous versions). If notes have been added to a file, PetWin automatically displays these when the file is opened. This greatly improves the utility of the Notes Editor and facilitates knowledge transfer.
- Table column widths are automatically resized to fit headings in the Album.
- User-defined Hydraulic Retention Time (HRT) calculators are now available. Users can select flowsheet elements to define the volume and flowrate terms for an HRT calculation. Multiple HRT calculators can be defined. Defined HRTs also can be plotted in the PetWin Album as a time series.
- The upper limit on the settling parameter V_0 has been significantly increased to facilitate simulation of ballasted activated sludge settling.
- The State Variable influent element now offers the same functionality for automatic filling of blank rows as with other influent elements.
- Groupings to assist in finding element specific items for tables and charts. Group titles are numbered and each group is sorted alphabetically.
- **Report to Word** is now directly accessible from the **File** menu.
- Several parameters related to nitrogen removal (*i.e.* deammonification rates, nitrification rates, and denitrification rates) have been made available for display in the PetWin Album in tables and/or charts. Additionally, for media-type bioreactors, these parameters are also calculated on a unit media area basis.
    - There is now a Common tab under **Project** > **Parameters** > **Kinetic**. This tab groups kinetic parameters that are not specific to one class of organism.
- Henry's Law coefficients are now shown in scientific notation format, allowing display of additional significant figures.

- PetWin alerts users if they have disabled metal reactions and attempt to run a simulation for a flowsheet containing one or more metal addition elements.
- If a user specifies an air supply rate for a bioreactor-type element, PetWin will ***automatically*** turn on the required oxygen modeling option.
- PetWin will alert the user that no model has been specified if a user does not select either PetWin's default biological model or their own user-defined Builder model.
- Improved display of the model stoichiometry matrix.
- Restructuring of the Help.
- New additions to the cabinet examples.
- Influent elements remember 'low' flow unit settings.
- Comma display for thousand separators.
- Expanded copy/paste/print facilities in state vectors.
- Total N reported in Explorer.
- Improved interpretation of "Mass rates" for element specific variables.
- Tabulation and plotting of model process rates in bar or time series charts.
- Exporting individual chart data to various formats from the right-click menu.
- Enhanced Chart Master settings. Specify defaults for current value and time series plots independently as well as default tools. [In Chart Master double-click the plot on the New chart template tab].
- Formatted charts for reporting nitrous oxide outputs (current values or time series).
- Model Builder usability improvements include:
  - An improved layout.
  - A cabinet of examples has been added (eg. ASM1, ASM2d, ASM3).
  - A recently used files list and a notes section to document your Builder files.
  - A simplified procedure for loading and saving .mod and other recognized file formats.