Model Developer

GPS-X 8.0

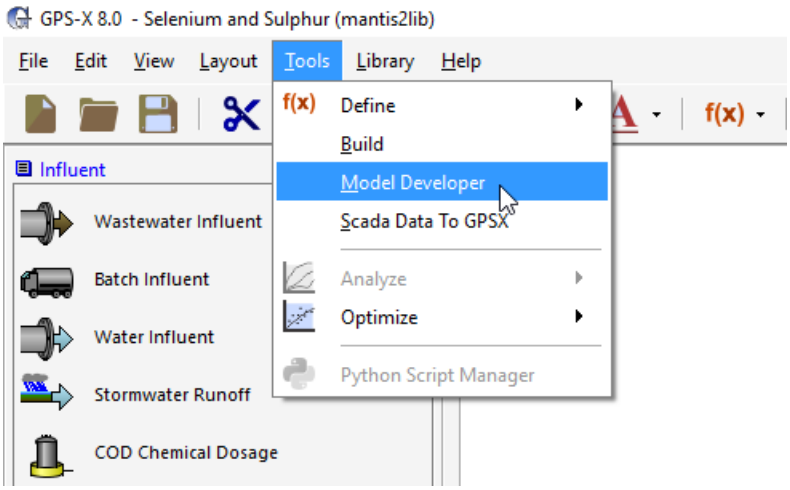
GPS-X Model Developer Tool

1. Background

Model Developer is a utility that allows GPS-X users to create and edit their own models in GPS-X. This model development makes use of the model matrix format for model specification, which is the standard format in the wastewater modelling literature. For more information on model matrix notation, please consult the IWA report on the structure of the ASM1 and ASM2d activated sludge models (Henze, *et al.,* 1987, and Henze *et al.,* 1998, respectively).

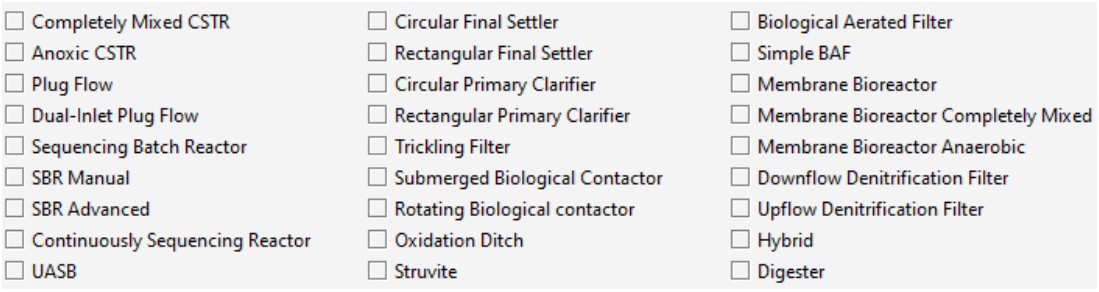
This document provides instruction on how to use Model Developer (MD), and assumes the user is familiar with mechanistic dynamic activated sludge models, and the matrix notation format.

Model Developer is accessed from the GPS-X Tools menu.



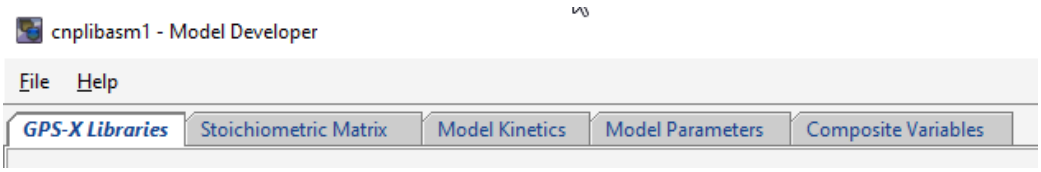
2. MD Components

MD is a application within GPS-X that organizes model content into a series of pages that contain information on model structure, parameters, and GPS-X variables. These pages are used, along with templates found in each GPS-X library, to create a biological model that is written for following GPS-X unit process objects:



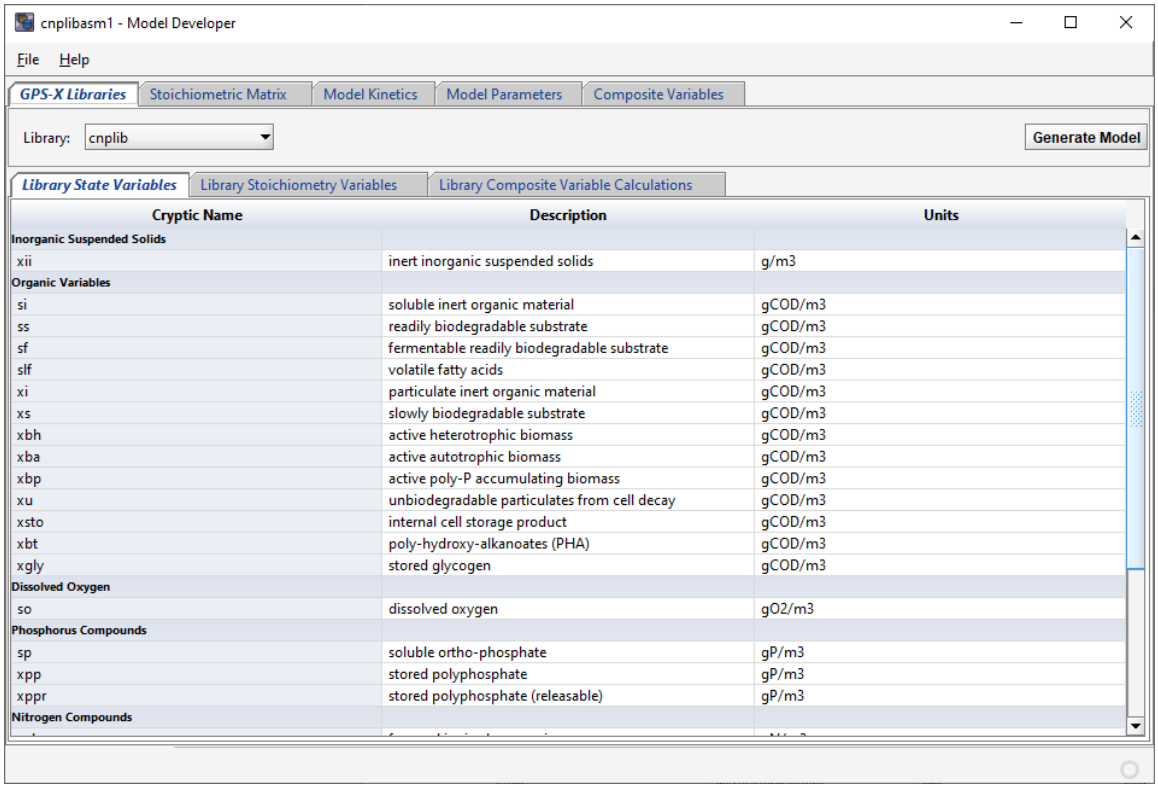
In each case, the biological model is implemented with the appropriate physical characteristics and hydraulic configuration appropriate to that object.

There are 5 sections to the Model Developer Tool, accessible through tabs at the top of the MD window: GPS-X Libraries, Stoichiometric Matrix, Model Kinetics, Model Parameters, and Composite Variables.



GPS-X Libraries

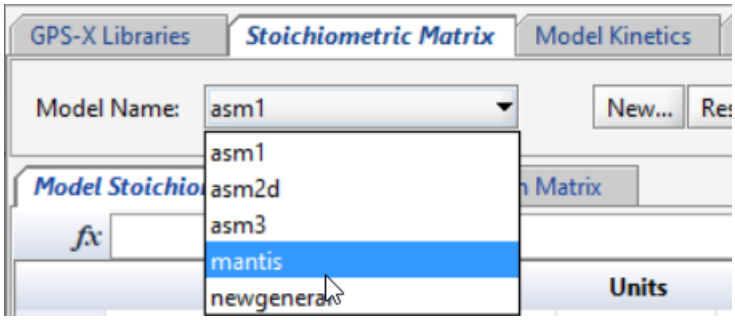
The GPS-X Libraries page shows information on the existing set of state variables and composite variable stoichiometry parameters in the GPS-X libraries, as well as the library-specific composite variable calculations. These are not changeable. Models can be made up of a full set or subset of the state variables shown on these pages. Select the appropriate library (from the **Library:** pull down menu) to display the state variable and composite stoichiometry set, and composite variable calculations.



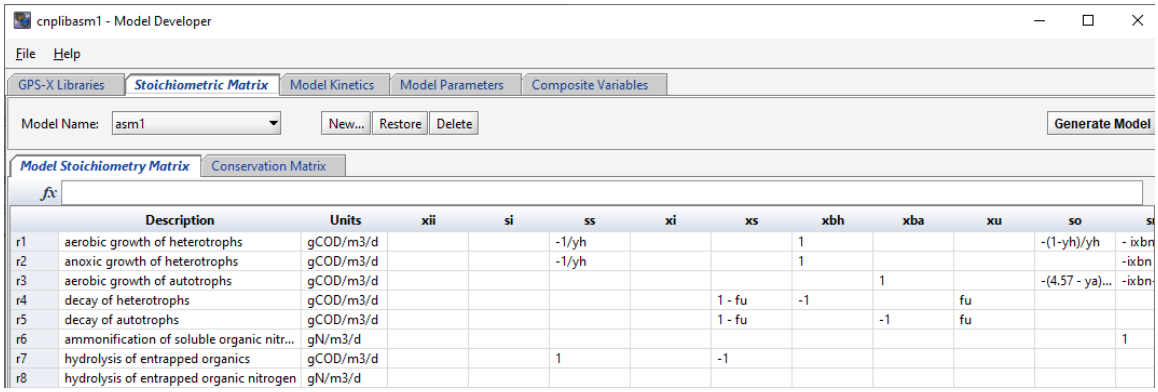
Cryptic Name	Description	Units
Inorganic Suspended Solids		
xii	inert inorganic suspended solids	g/m3
Organic Variables		
si	soluble inert organic material	gCOD/m3
ss	readily biodegradable substrate	gCOD/m3
sf	fermentable readily biodegradable substrate	gCOD/m3
slf	volatile fatty acids	gCOD/m3
xi	particulate inert organic material	gCOD/m3
xs	slowly biodegradable substrate	gCOD/m3
xbh	active heterotrophic biomass	gCOD/m3
xba	active autotrophic biomass	gCOD/m3
xbp	active poly-P accumulating biomass	gCOD/m3
xu	unbiodegradable particulates from cell decay	gCOD/m3
xsto	internal cell storage product	gCOD/m3
xbt	poly-hydroxy-alkanoates (PHA)	gCOD/m3
xgly	stored glycogen	gCOD/m3
Dissolved Oxygen		
so	dissolved oxygen	gO2/m3
Phosphorus Compounds		
sp	soluble ortho-phosphate	gP/m3
xpp	stored polyphosphate	gP/m3
xppr	stored polyphosphate (releasable)	gP/m3
Nitrogen Compounds		

Stoichiometric Matrix

The Stoichiometric Matrix tab shows the model matrix for all models available. You can select the appropriate model from the **Model Name:** drop down menu.

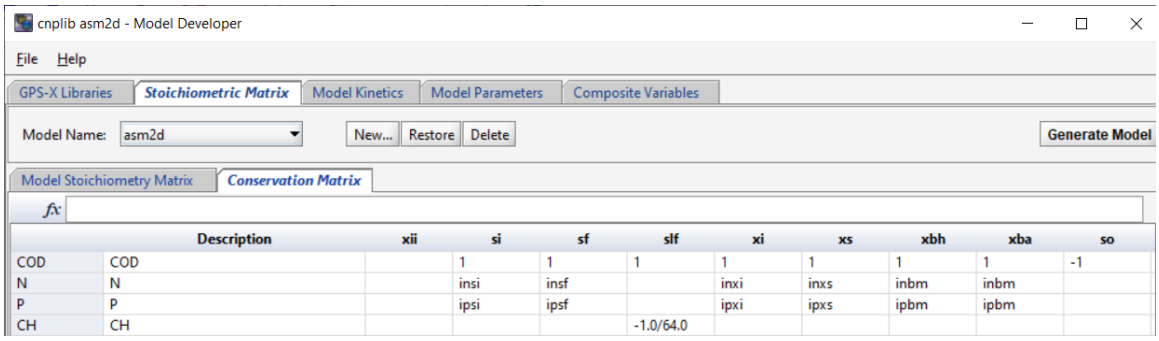


The Model Stoichiometry tab shows the model matrix, with state variables in columns and kinetic processes in rows. Textual descriptions of the kinetic processes are shown on the left.



	Description	Units	xii	si	ss	xi	xs	xbh	xba	xu	so	s
r1	aerobic growth of heterotrophs	gCOD/m3/d			-1/yh			1			-(1-yh)/yh	- ixbn
r2	anoxic growth of heterotrophs	gCOD/m3/d			-1/yh			1				-ixbn
r3	aerobic growth of autotrophs	gCOD/m3/d							1		-(4.57 - ya)...	-ixbn-
r4	decay of heterotrophs	gCOD/m3/d					1 - fu	-1		fu		
r5	decay of autotrophs	gCOD/m3/d					1 - fu		-1	fu		
r6	ammonification of soluble organic nitr...	gN/m3/d										1
r7	hydrolysis of entrapped organics	gCOD/m3/d			1		-1					
r8	hydrolysis of entrapped organic nitrogen	gN/m3/d										

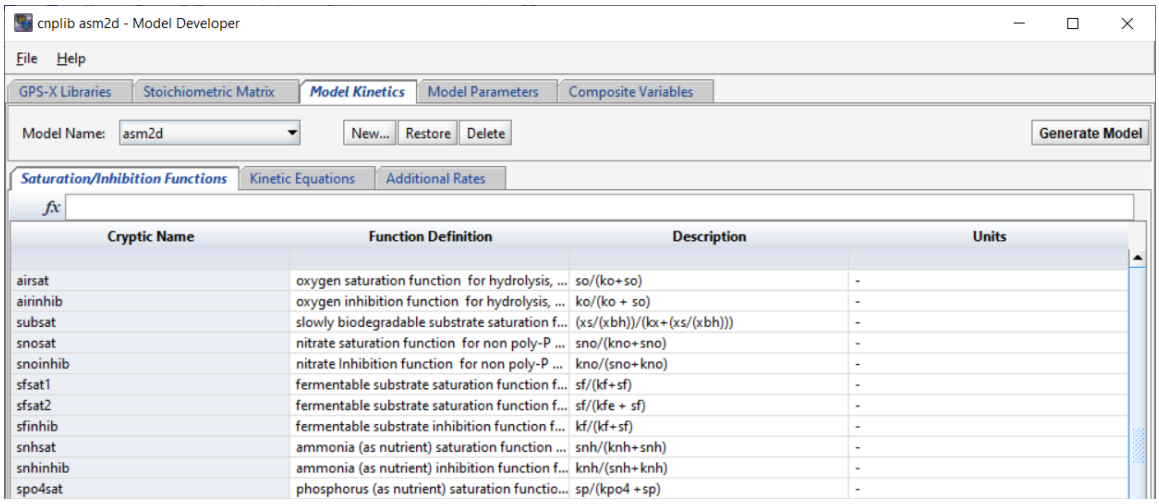
The Conservation Matrix tab shows the elements of the conservation matrix, used to calculate unknown model stoichiometry via mass balance. For more information on using conservation matrices, please see the ASM2d report. The element in the model stoichiometry table that will be calculated from the conservation matrix is filled with the symbol @{var}, where {var} represents the element being conserved, as shown in the left column of the conservation matrix (e.g. @COD).



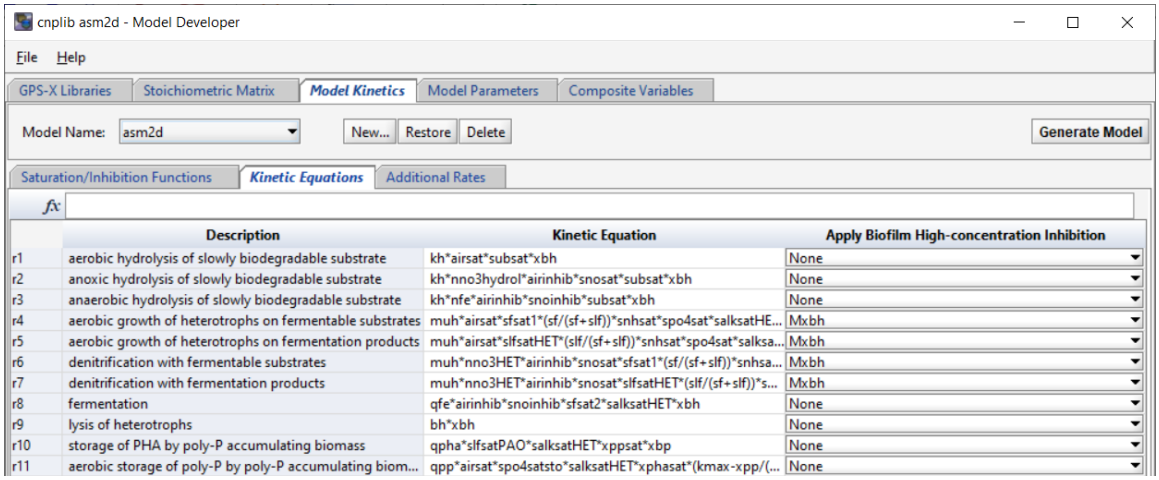
	Description	xii	si	sf	slf	xi	xs	xbh	xba	so
COD	COD		1	1	1	1	1	1	1	-1
N	N		insi	insf		inxi	inxs	inbm	inbm	
P	P		ipsi	ipsf		ipxi	ipxs	ipbm	ipbm	
CH	CH				-1.0/64.0					

Model Kinetics

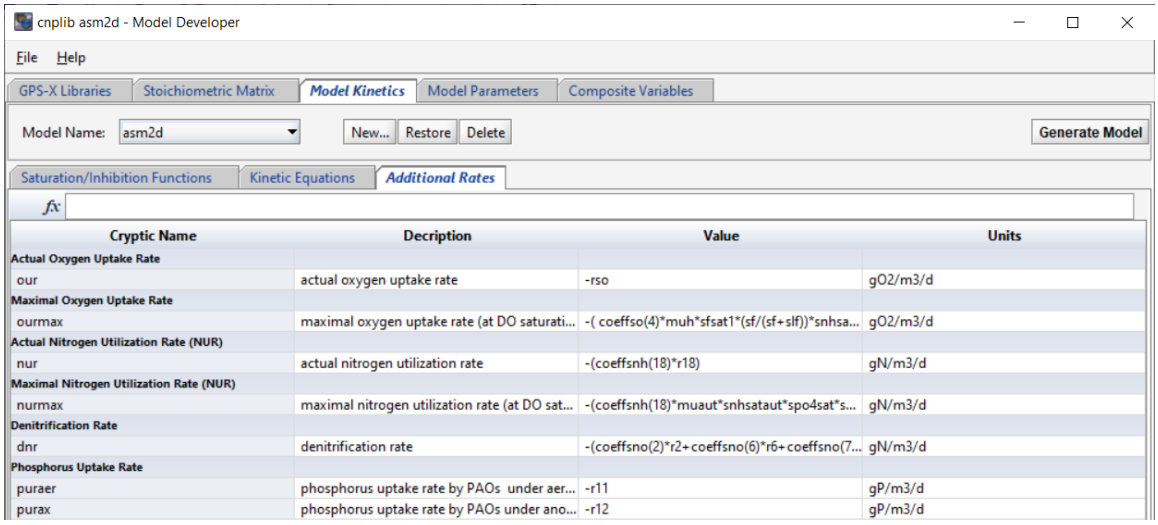
The Model Kinetics page contains information on the kinetic process rates used in the model (which are represented by rows in the model stoichiometry matrix). The Saturation/Inhibition Functions tab shows all saturation and inhibition functions used in the creation of the kinetic process rates. Each variable is shown with its corresponding equation and units.



The “Kinetic Equations” tab shows the kinetic equations themselves. The rates and descriptions match those shown on the model stoichiometry tab. The corresponding rate equations and units are shown and edited on this tab. If new rates are added to the stoichiometric matrix, new corresponding rows will show here as well. Any saturation functions that should be applied to the kinetic rates in the biofilm objects (only) can be selected from the drop-down menus in the right-hand column.



Any other additional equations that might be useful to calculate in all reactors can be added in the “Additional Rates” tab.



Cryptic Name	Decription	Value	Units
Actual Oxygen Uptake Rate			
our	actual oxygen uptake rate	-rso	gO2/m3/d
Maximal Oxygen Uptake Rate			
ourmax	maximal oxygen uptake rate (at DO saturati...	-(coeffso(4)*muh*sfsat1*(sf/(sf+slf))*snhsa...	gO2/m3/d
Actual Nitrogen Utilization Rate (NUR)			
nur	actual nitrogen utilization rate	-(coeffsnh(18)*r18)	gN/m3/d
Maximal Nitrogen Utilization Rate (NUR)			
nurmax	maximal nitrogen utilization rate (at DO sat...	-(coeffsnh(18)*muaut*snhsataut*spo4sat*s...	gN/m3/d
Denitrification Rate			
dnr	denitrification rate	-(coeffsno(2)*r2+coeffsno(6)*r6+coeffsno(7...	gN/m3/d
Phosphorus Uptake Rate			
puraer	phosphorus uptake rate by PAOs under aer...	-r11	gP/m3/d
purax	phosphorus uptake rate by PAOs under ano...	-r12	gP/m3/d

Model Parameters

The fourth tab of the MD tool (labelled “Model Parameters”) contains variables and parameters that are part of the model. Each variable/parameter is listed along with its descriptive name, value and appropriate units. This page includes:

- **State Variables:** the model state variables, and their initial values, and diffusion coefficients for biofilm objects.
- **Stoichiometric parameters:** both model stoichiometric parameters (from the Model Matrix, such as yield, etc.) and organic/nutrient fractions are listed here (e.g. N fraction of biomass).
- **Kinetic parameters:** model kinetic parameters are listed here, including values for 10C and 20C temperatures, or Arrhenius temperature coefficient.
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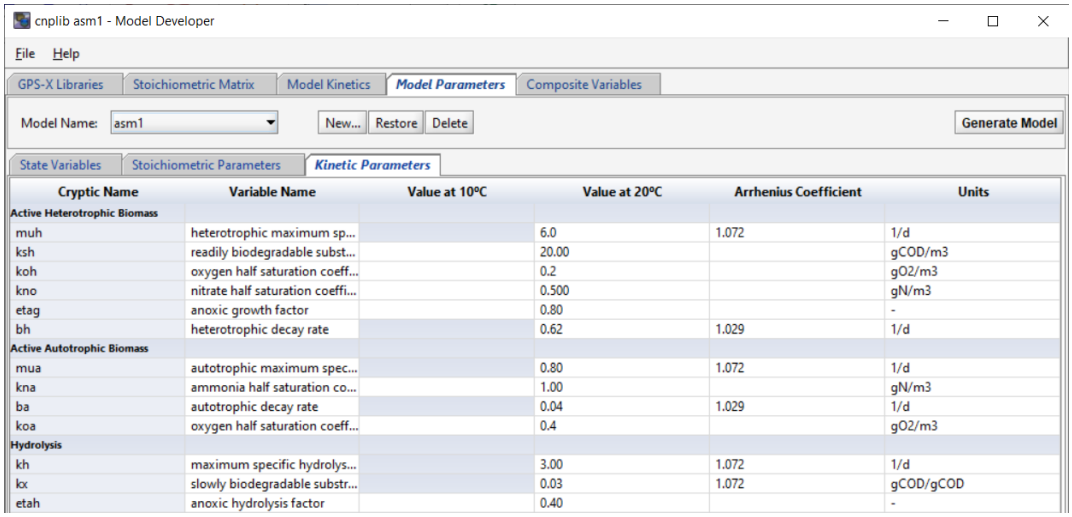


Cryptic Name	Variable Name	Value at 10ºC	Value at 20ºC	Arrhenius Coefficient	Units
Active Heterotrophic Biomass					
muh	heterotrophic maximum sp...		6.0	1.072	1/d
ksh	readily biodegradable subst...		20.00		gCOD/m3
koh	oxygen half saturation coeff...		0.2		gO2/m3
kno	nitrate half saturation coeffi...		0.500		gN/m3
etag	anoxic growth factor		0.80		-
bh	heterotrophic decay rate		0.62	1.029	1/d
Active Autotrophic Biomass					
mua	autotrophic maximum spec...		0.80	1.072	1/d
kna	ammonia half saturation co...		1.00		gN/m3
ba	autotrophic decay rate		0.04	1.029	1/d
koa	oxygen half saturation coeff...		0.4		gO2/m3
Hydrolysis					
kh	maximum specific hydrolys...		3.00	1.072	1/d
kx	slowly biodegradable substr...		0.03	1.072	gCOD/gCOD
etah	anoxic hydrolysis factor		0.40		-

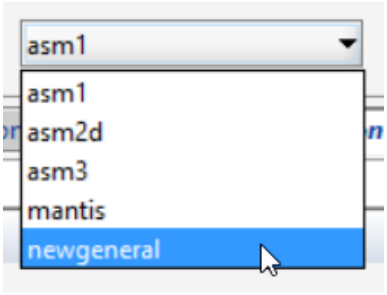
Note that if temperatures are entered for both 10C and 20C, the Arrhenius coefficient will be calculated from these values. Alternatively, you can enter just the 20C value, and enter an Arrhenius coefficient directly.

Composite Variables

The final tab on the MD page is the Composite Variable page, where the stoichiometry of the model is assigned to the fixed GPS-X composite variable stoichiometry. For example, GPS-X has a fixed variable name for the nitrogen fraction of particulate inert COD – inxi. These variable names and descriptions are shown in the first two columns, and are not changeable. If your model uses these model conventions, then you can select the appropriate value in the right-hand column. If you have nutrient fractions that are differently named than the fixed GPS-X variable set in the left column, then please select the appropriate variable name from the list. If you do not have an equivalent variable in your model for some of the standard GPS-X variables, you can set the GPS-X variables to zero.

3. Entering Models into Model Developer

The following 5 GPS-X activated sludge models are available in Model Developer by default.



To create a new model, select File > Save Model As… and save a the model with a new name in the c:/gps-x651/md/models/ folder.

You cannot generate models that have the same name as an existing model in GPS-X – if you wish to regenerate a new, modified version of asm1 (for instance), you will have to give it a new name. This is done to protect the existing library structure.

There are 3 steps involved in preparing a model in MD:

1) Entering/editing the model stoichiometric matrix

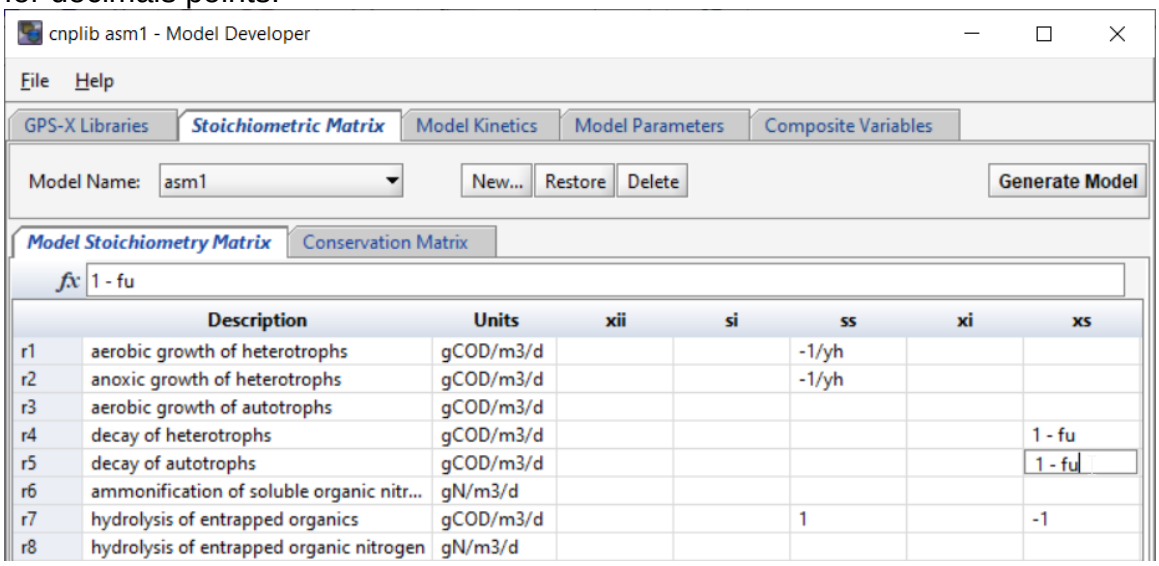
2) Writing the kinetic rate equations (including any internal saturation/inhibition functions) and any other supplemental kinetic rate equations if interest

3) Entering model parameters and default values

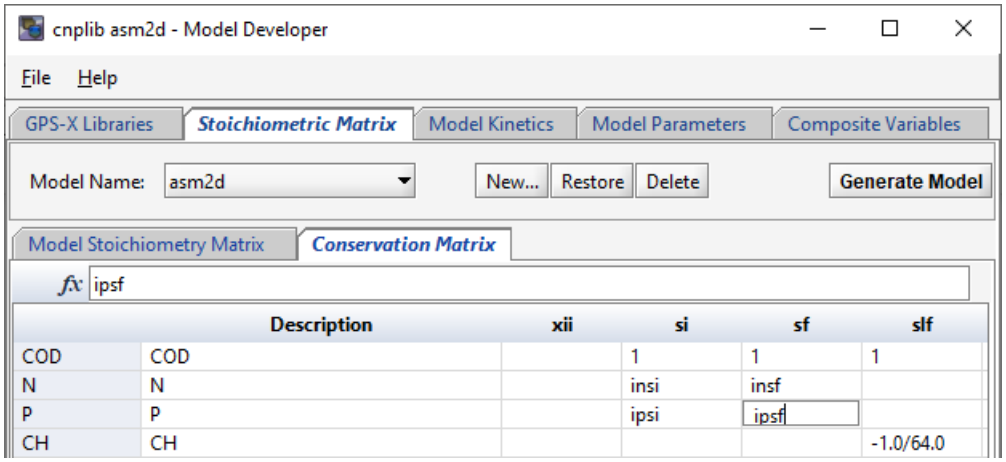
Specifying the model in the model stoichiometric matrix

The model matrix is specified in Model Stoichiometry page. New state variables may be added to the model (provided they are part of the GPS-X library) by right-clicking on a column, and selecting a new state variable from the available list. New rates are added by right-clicking on the matrix and adding a new row.

Model stoichiometric relationships can be entered directly into each cell of the matrix by clicking on the appropriate cell, and entering in the equation. Include a decimal place with all real values (including integers), when entering stoichiometric equations. Please note that MD does not support using commas for decimals points.



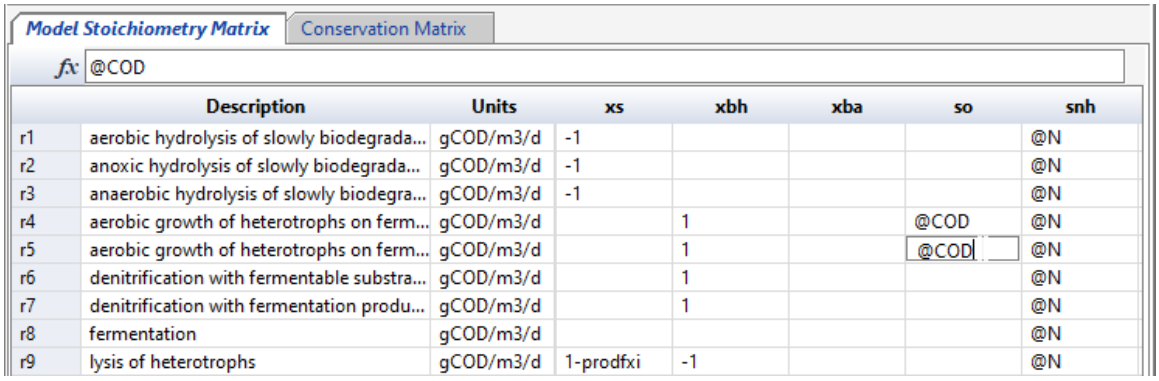
The conservation matrix (shown on the conservation matrix tab) may be incorporated by entering values in the matrix that indicate which conservation element is used. For details of using a conservation matrix, please refer to the ASM2d model publication (Henze, *et al*., 1998).



The nomenclature to be used in the cell for which the stoichiometry is to be calculated is shown below:

@COD – stoichiometric constant for the current row, based on COD conservation

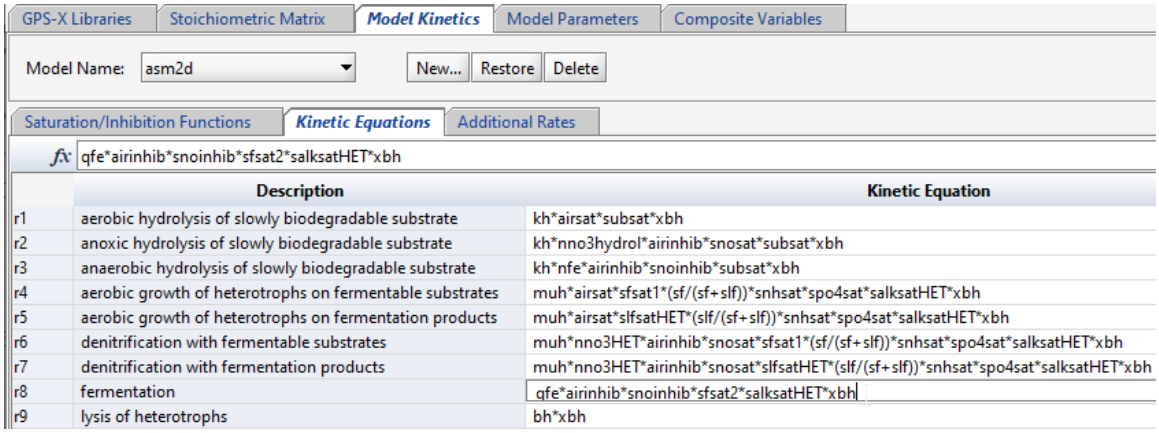
Each stoichiometric constant that is determined from the conservation matrix must use only one of the conservation elements available (e.g. COD, above). Each conservation element is listed in a separate row in the conservation matrix, and contains the appropriate stoichiometry for each state variable. For a good example of the use of the conservation matrix, please see the ASM2d model in MD.



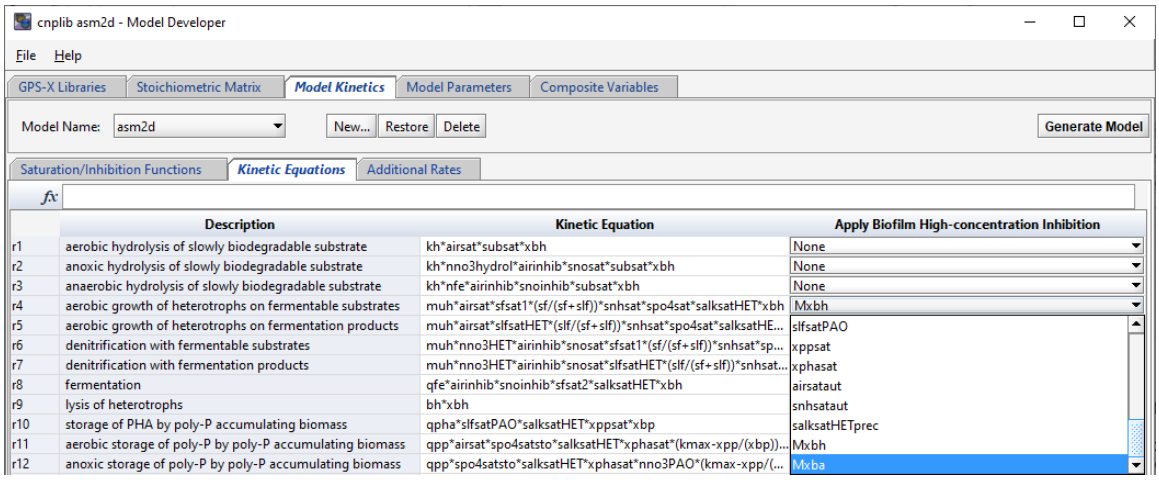
Entering Kinetic Rate equations

On the Model Kinetics page, on the Kinetic Rates tab, the kinetic rate equations for each row of the matrix are shown. The descriptive name of the rate is shown here as well, along with the units.

If the rate equation contains terms that would be useful to have calculated separately (such as inhibition or saturation functions), those can be listed (along with descriptive names) in the “Saturation/Inhibition Functions” tab.



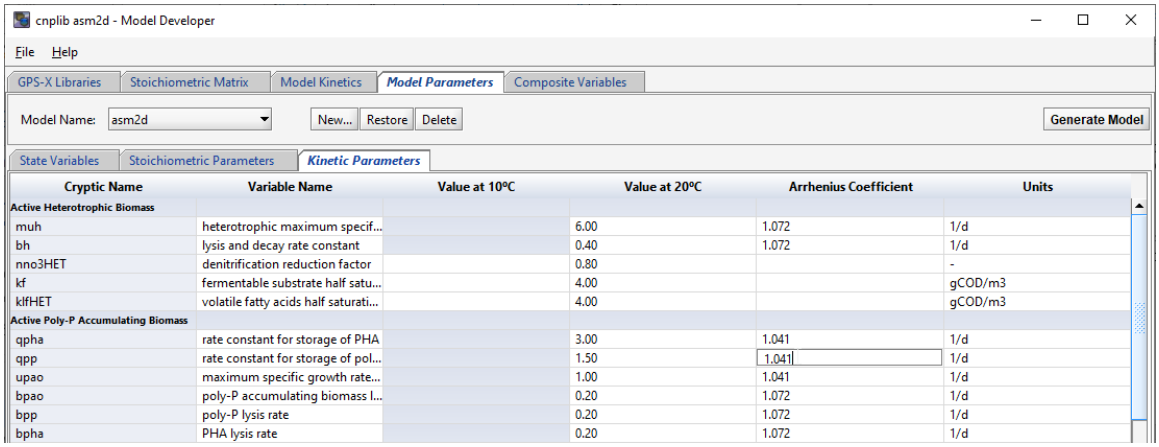
The “Apply Biofilm High-Concentration Inhibition” term on the right hand side is a feature that allows a saturation term (which must first be defined on the Saturation/Inhibition Functions tab) to be applied to only the biofilm models in GPS-X (hybrid, denitrification filters, BAF, simple BAF, trickling filter, RBC and SBC). This allows high-concentration inhibition terms to be applied to the appropriate growth equations (in biofilm objects only). Select the appropriate inhibition term from the drop-down menu.



Entering model variables and parameters

On the “Model Parameters” page, enter all of the model stoichiometry in the “Stoichiometric Parameters” tab. Right-click on a row to add new parameters, if required.

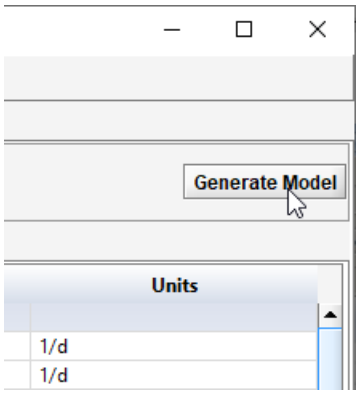
Next, click over to the “Kinetic Parameters” tab, and enter the parameters of the model and their values and units. If the parameter is temperature sensitive, you can list values for 10C and 20C, or Arrhenius coefficient. Right-click on a row to add new rows if required.



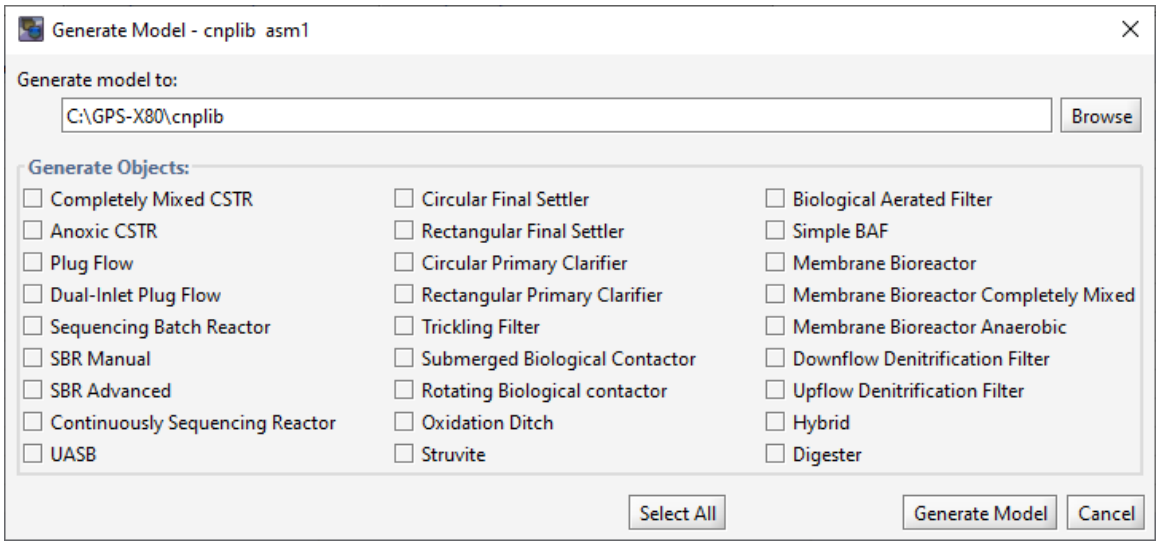
4. Generating Models

Once the matrix and all other tabs have been filled out, the model can be generated. Note that the model will be generated for the library showing in the Library: pull-down menu on the GPS-X Libraries page.

The model is generated by pressing the “Generate Model” button, as shown below.



You will be prompted to enter the full path to the GPS-X library where the new model will be written (and where the template files are – which are the same by default), as shown below:



Once you've entered the appropriate paths, you can select which unit processes should be generated (plug flow, MBR, etc.). Use the "Select All" button to generate models for all objects. MD will write out the files containing all the models. This may take up to a minute, depending on the speed of the computer.

Once the models have been written, close MD, and restart GPS-X. Select the library where the new models were written from the pull-down library menu at the top of the GPS-X screen.

When you select one of the objects listed section two (CSTR, plug flow tank, etc.), you will see the new model available under the Models menu.

5. A Note about Using Your New Models

Because your new model is not part of the original GPS-X structure, you will not be able to select it from the "Biological Models" menu in the influent object menu, and the Influent Advisor tool will not be available for your model. We recommend using the STATES influent model to simplify influent characterization when using custom biological models.

6. Technical Support/Troubleshooting

If you have any difficulties using Model Developer, or properly incorporating the models into GPS-X, please contact us at support@hydromantis.com.

7. References

Henze M, Grady C P L, Gujer W, Marais G v R and Matsuo T (1987). Activated sludge model no. 1. IAWPRC Scientific and Technical Report No. 1, IAWPRC, London.

Henze, M., W. Gujer, T. Mino, T. Matsuo, M.C. Wentzel, G.v.R. Marais and M.C.M. van Loosdrecht. (1998). Outline - Activated sludge model no. 2d. Proceedings of the Specialized Conference on Modelling and Microbiology of Activated Sludge Processes, Kollekolle, Denmark, 16-18 March.

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