

# THE EPSILON GROUP

# SAAM II

## WHAT'S NEW IN VERSION 2.1?

### INTRODUCING VERSION 2.1

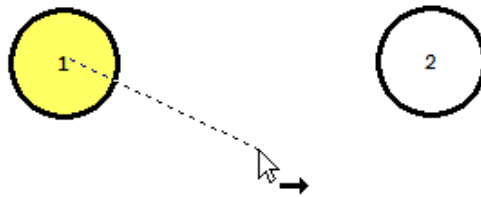
The Epsilon Group (TEG Virginia), which licensed SAAM II from the University of Washington in June of this year, is pleased to announce the release of Version 2.1 of SAAM II. This new version implements some enhancements to the software requested by users in the recent survey from the University of Washington. TEG requests your feedback on how these enhancements have been implemented. We also ask you to check the SAAM II website as we feel it is important to keep users abreast of what is being planned and designed for future enhancements.

### CHANGES TO THE SAAM II TOOLBOX

A small but helpful change has been made to the SAAM II Toolbox. For example, When constructing your model using the Model Building tools, to create a transfer you had to click first on the FROM compartment, and then click on the TO compartment. Sometimes if you didn't click correctly in the TO compartment you would get, for example, an INPUT arrow.

Version 2.1 permits you to "click and drag" when creating transfers. That is, you click on the FROM compartment, and while you can still click on the TO compartment, you can also drag to the TO compartment.

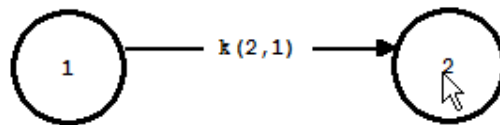
When you click on the FROM compartment, it becomes highlighted. If you hold the mouse key down and draw towards the TO compartment, a dotted line will appear together with the cursor (with the TRANSFER arrow so you know TRANSFER is active) as shown in the example below:



When you arrive at the TO compartment, it becomes highlighted with the dotted line connecting the FROM and TO compartments as shown in the example below.



When you release the mouse button, the transfer will be complete as shown in the example below.



## CHANGES TO PLOTTING AND TABLES SETTINGS

There are new features on the SAAM II Toolbar. The old bar was:

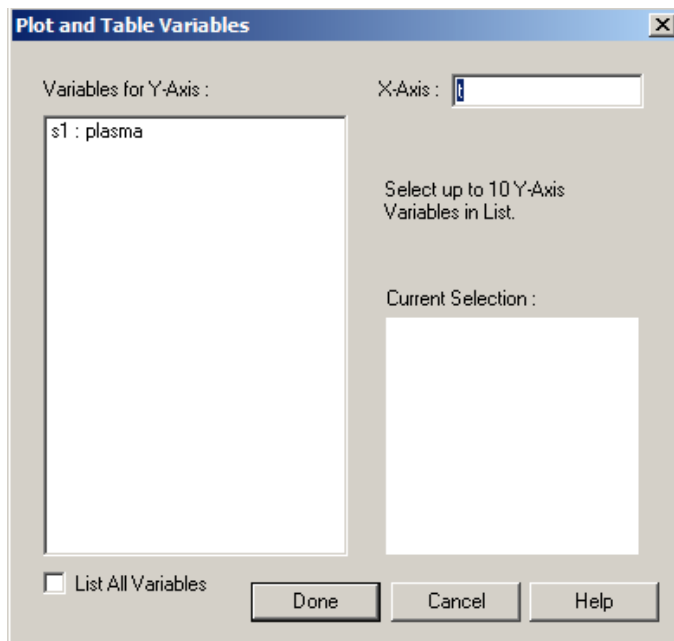


The new SAAM II Toolbar is:

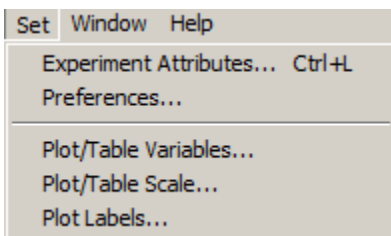


You will notice dimmed tools between the **FIT** and **TOOLBOX** tools. When a Plot is open and active, these tools will not be dimmed, and will access **PLOT/TABLE VARIABLES**, **PLOT/TABLE SCALE** and **PLOTLABELS** without having to go to the **SET** menu.

When you select the **PLOT** tool, the **Plot and Tables Variables** dialog box will open:



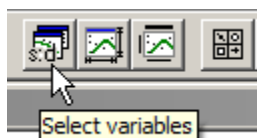
As the PLOT tool is active, and you can change the variables, scale and labels using the commands in the SET menu:



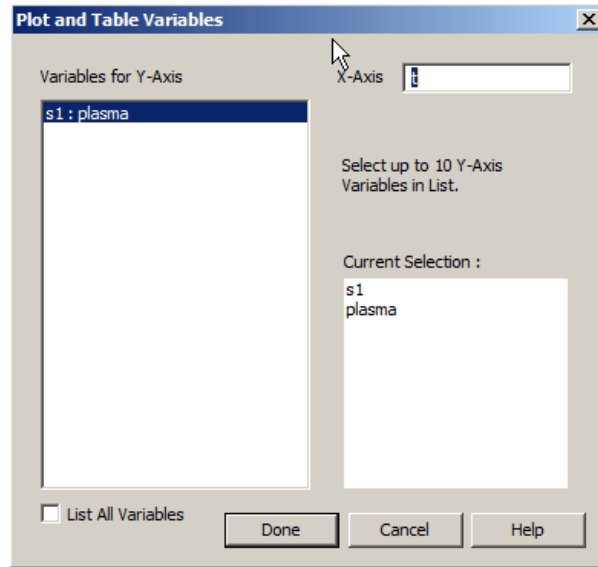
This was cumbersome, and in Version 2.1 there are two quicker ways to access these. One is to right click on the plot; the options shown in the SET menu above will open. The other way is to use the new Tools that have been implemented on the SAAM II Toolbar:



With PLOT active, the tools following the FIT tool are active (as shown above, they are dimmed when PLOT is not active). These tools permit you to open PLOT AND TABLE VARIABLES, PLOT AND TABLE SCALE, and PLOT LABELS dialog box quickly:



That is, if you click on the Select variables tool, the PLOT AND TABLE VARIABLES dialog box will open:



Similarly, with the other two new tools, you can check these out in the Plotting Tutorial on the SAAM website.

If instead of a plot you open a TABLE, the PLOT AND TABLE VARIABLES and PLOT AND TABLE SCALE dialog tools are available. The PLOT LABEL tool is not available as, in a Table, there is nothing to label.

## CHANGES TO IMPORTING AND EXPORTING PLOTS AND TABLES

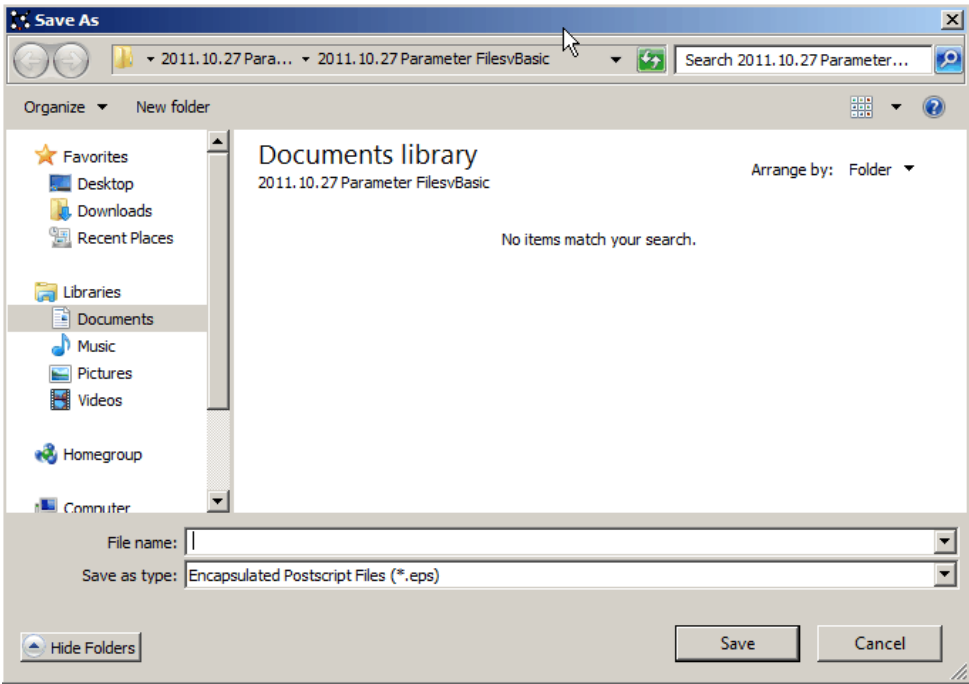
You can now easily export plots to an encapsulated post script (\*.eps) file or an enhanced metafile (\*.emf), or copy and paste a plot directly into a WORD document. You can also export tables to a comma separated values (\*.csv) file.

### *Exporting plots*

Suppose you have a Plot open in your SAAM II run. If you right-click on the Plot, the following dialog box will open:



Two new options are available in this dialog box: Copy and Export plot ... If you select Export Plot, the Save As dialog box will open:



You can then choose where you want to save the file, and you can save it as an \*.eps file or an \*.emf file.

If you choose “Copy”, the plot as shown on your Drawing Canvas will be copied, and you can “Paste” it directly into, for example, a WORD document.

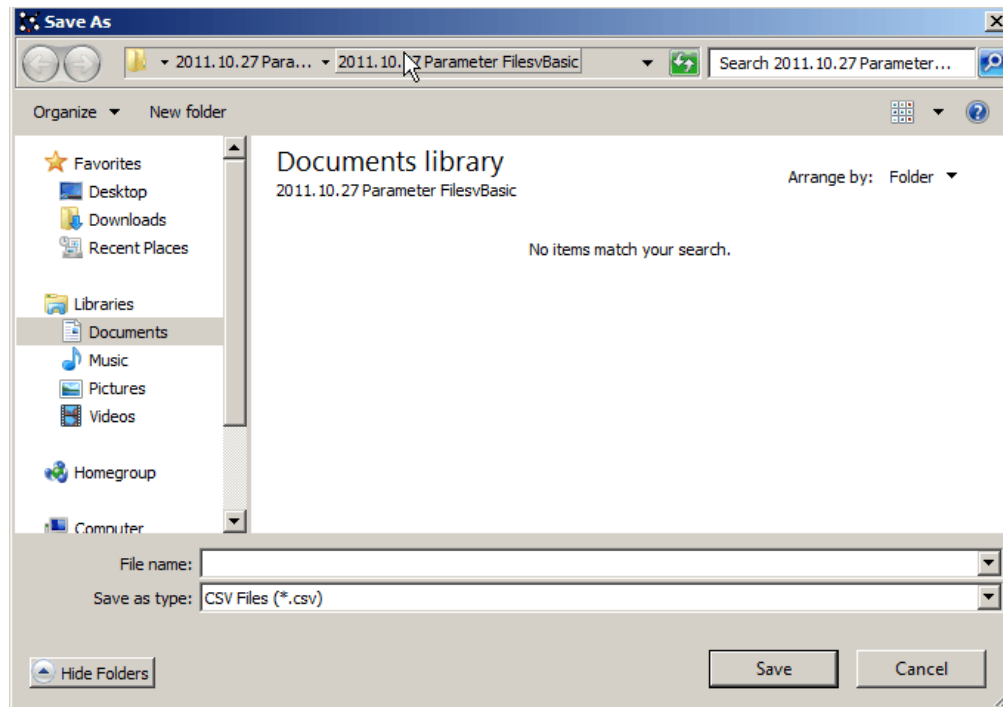
“Export plot” can also be accessed from the FILE menu.

*Exporting tables*

If you have a Table open and active on your Drawing Canvas, you can copy it to a .csv file. In the File menu:

New	Ctrl+N
Open...	Ctrl+O
Close	
Save	Ctrl+S
Save As...	
Export table (CSV)...	
Print...	Ctrl+P
Print One Copy	Ctrl+1
Print Preview	
Print Setup...	
Page Setup...	
Exit	Alt+F4

if you click “Export table (CSV)”, the Save As dialog box will open:

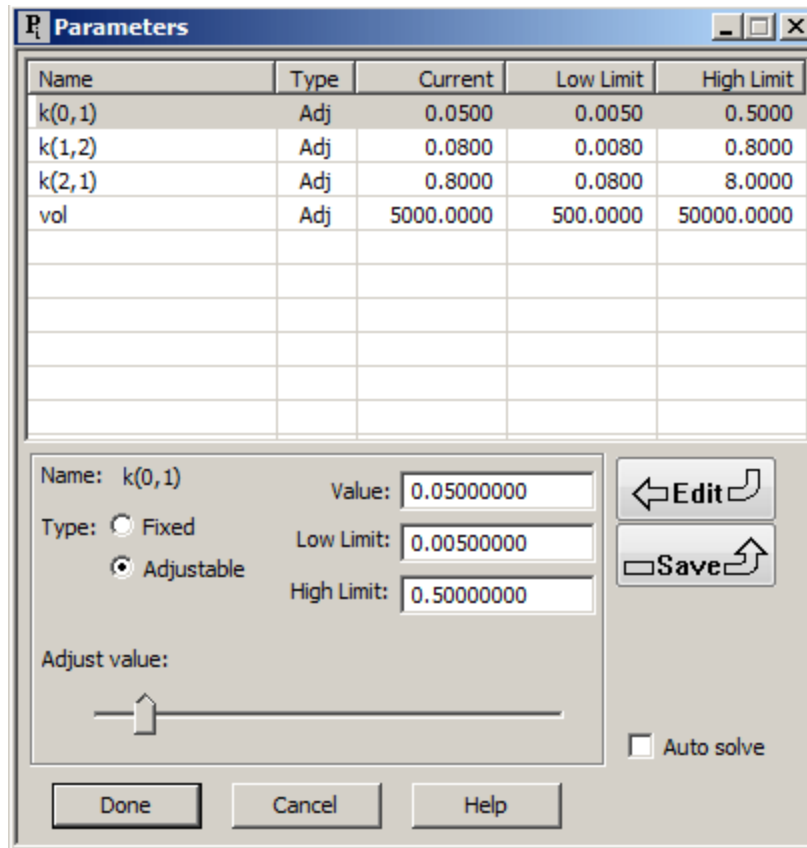


You can save your table as a \*.CSV file which can be opened directly in Excel.

## THE PARAMETER SLIDER BAR

For years, many users have requested a means by which to hand-fit data more quickly than having to open the Parameters Dialog box to change a particular parameter value. In addition, they would like to have a feature to do a “poor man’s” sensitivity analysis, i.e. to see how sensitive a solution is to a change in a parameter value.

To accomplish this, in version 2.1 TEG has implemented a slider bar in the Parameters Dialog box. In addition, when the Parameters dialog box is opened, notice also the lines and columns in the Parameters window which make it easier to read the values for the different parameters:



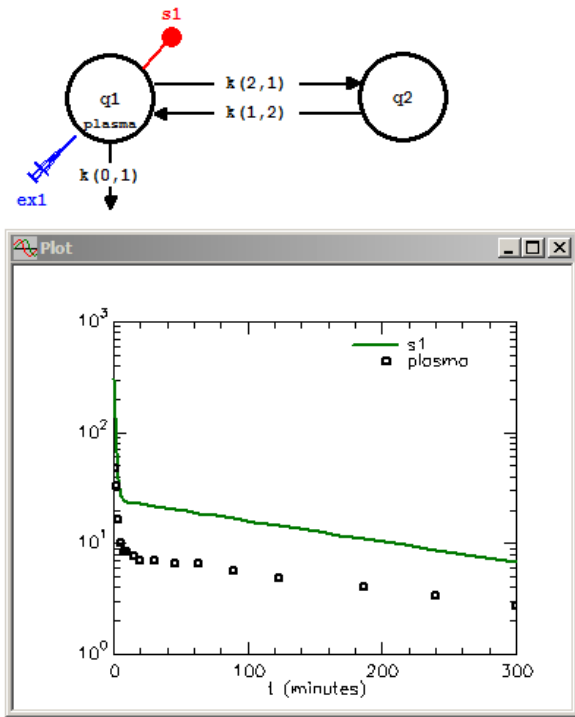
The slider bar, Adjust value, is near the bottom of the dialog box. As illustrated below, the adjustment tool on the Adjust value slider bar moves, for each parameter, between the Low Limit and High Limit.

There is an Auto solve check box.

- If this check box is not checked, then when a new parameter value is chosen on the Adjust value slider bar, you will have to SAVE it, and then click SOLVE in order to solve with that new value.
- If this check box is clicked, then when you move to a new value, SAAM II will automatically SOLVE. If the PLOT window is open, the plot will be updated.

The Adjust value slider bar is now an integral part of the Parameters dialog box. Why? Why isn't it just a tool that can be requested by the user? The reason is that the Adjust value slider bar permits a very rapid way to hand-fit your data!! That is, you can quickly hand-adjust parameter values to improve upon your initial estimates. Hand fitting your data in this manner is the best way to learn how your model and data interact, i.e. you will learn which parameter affects certain parts of the solution. This is a highly recommended exercise for all who model, especially with new data sets.

As an example, consider the following:



**Parameters**

Name	Type	Current	Low Limit	High Limit
k(0,1)	Adj	0.0500	0.0050	0.5000
k(1,2)	Adj	0.0800	0.0080	0.8000
k(2,1)	Adj	0.8000	0.0800	8.0000
vol	Adj	5000.0000	500.0000	50000.0000

Name: vol Value: 5000.00000000

Type:  Fixed  Adjustable

Low Limit: 500.00000000 High Limit: 50000.00000000

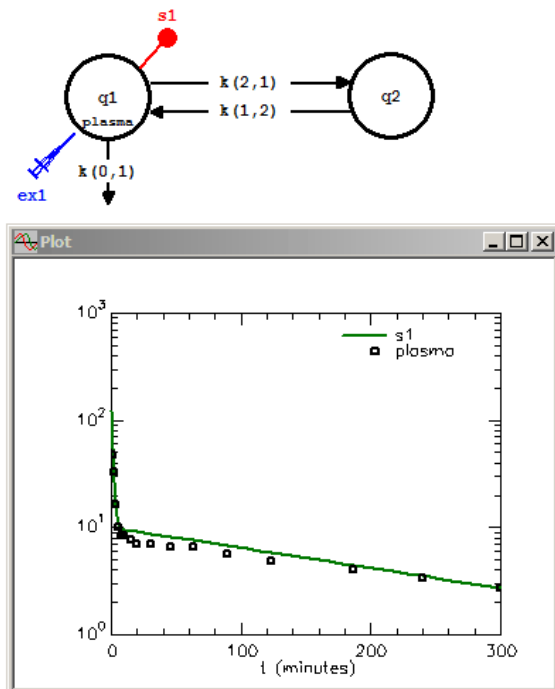
Adjust value:

Auto solve

Done Cancel Help

This is the solution to the two compartment model with the values shown in the Parameters dialog box. While the shape of the curve is okay, the scale factor vol is off; it needs to be a little larger so as to lower the predicted value.

If you click the Auto solve check box, be sure vol is the selected parameter (as it is above), and move the slider bar to 12380, when you release the slider bar:



**Parameters**

Name	Type	Current	Low Limit	High Limit
k(0,1)	Adj	0.0500	0.0050	0.5000
k(1,2)	Adj	0.0800	0.0080	0.8000
k(2,1)	Adj	0.8000	0.0800	8.0000
vol	Adj	12380.0000	500.0000	50000.0000

Name: vol Value: 12380.00000000

Type:  Fixed  Adjustable

Low Limit: 500.00000000 High Limit: 50000.00000000

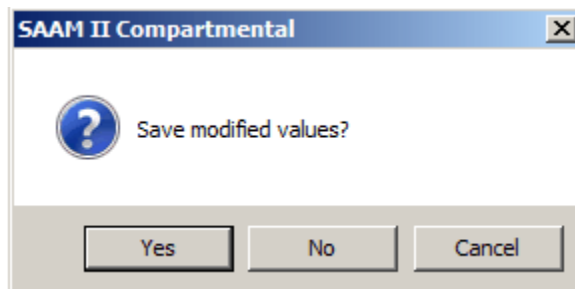
Adjust value:

Auto solve

Done Cancel Help

The solution is updated with the current value. It should be noted with the cursor on the slider tool, you can nudge the value with the left and right hand arrows on the keyboard.

When you click Done in the Parameters dialog box,



will appear, and you can check Yes, No, or Cancel. If you just close the Parameters dialog box by clicking in the upper right-hand corner, the new value will be automatically saved.

The question arises: when using the parameter slider bar, can I compare new solutions to a “baseline” solution. The answer is “yes”; it requires using SAAM II “Save Solutions” tool (this is explained in more detail in the Basic Parameters tutorial. Basically you can use the “Save Solutions” tool to create a baseline solution. Once you solve your model with another parameter value, you can plot this solution and include your “baseline” solution in the plot. Then whenever you change a parameter value using the parameter slider bar and SOLVE, the plot will automatically be updated with the new solution plotted along with the “baseline” solution.

There are enhancements to how the slider bar functions that can be made; TEG would like your feedback on what additions or changes you would like to see.

## WHAT'S NEXT?

The Epsilon Group is in the process of designing new features for SAAM II, and invites you to watch the website for progress, and to make comments or provide feedback so that the implementation will help you in your modeling work. If you have enhancements you would like to see added to the list, please contact The Epsilon Group: [saam2support@tegvirginia.com](mailto:saam2support@tegvirginia.com).

Here is what is coming in the next few months:

- Batch processing. You will be able to analyze data from several experiments on the same system in batch mode. Specifically, you will be able to have your experimental data for each subject either in individual files or one large file. You will then add a few lines to the individual data files to specify things like the amount of a dose in an experimental input.

To access SAAM II BATCH, you will open a study file which will be a “reference” file. Those who have used PopKinetics will recognize the “reference” file. The “reference” file will specify the model to be used including the experimental protocol (but not amounts so, for example, the dose amount can vary).

SAAM II BATCH will analyze your expanded data file, create individual study files (which you will have the option to save for other work), SOLVE or FIT for each, produce output information for each, and have the option of post-process in PopKinetics.

- Automatic differentiation. This is a computational enhancement. In order to integrate and optimize (SOLVE and FIT), SAAM II has to create derivatives. Currently there are two methods available which, at the time SAAM II was created until recently, were state-of-the-art. The methods are the forward and central difference. The forward difference is fast but not as accurate as central difference. Currently to obtain the most accurate parameter estimates and their errors, the User should FIT first with the forward difference, and then one last FIT with the central difference. Which method is used is set in the COMPUTATIONAL SETTINGS dialog box.

A new method which calculates the derivatives is called automatic differentiation. The person responsible for SAAM II's numerical algorithms has been involved in developing this theory, and TEG plans to implement this method as the default in SAAM II as it is quicker and more accurate. (For more information, <http://www.coin-or.org/CppAD/> )

- With the advent of Windows 7 it is much easier to implement parallel processing. Although in the vast majority of cases the computations in SAAM II are sufficiently fast, there are some really large models being created whose solution time in SAAM II is slow. This happens because of the way in which integration and optimization is performed in SAAM II; as most of you know, it is extremely robust and accurate.

As a result of comments from the users who develop large models, and in anticipation of where biomedical/pharmaceutical modeling is going, TEG is planning to implement a parallel processing capability in SAAM II.

Please stay tuned to our website for SAAM II updates!!!