Using SAAM II

Working with Tables

Working with Tables

Prerequisites

The prerequisite for this tutorial is having worked through the SAAM II introductory tutorial, "Getting Started with **SAAM II Compartmental**."

What you will learn in this tutorial

The purpose of this tutorial is to show you how to use Tables to export information from SAAM II to other applications. You will learn

- How to export information to a plotting application (Part 1)
- How to export the residuals and weighted residuals (Part 2)

Files Required

Study Files: The study file for this tutorial is

study_0.stu

This file is included as part of this tutorial. This file is the same as **study_0.stu** that is installed in the SAAM II program folder and referred to in the **SAAM II** User Guide.

Introduction

This tutorial focuses on how to use tables that can be created by SAAM II. Many users want to post-process results from SAAM II. This can include using other graphics packages or statistical packages.

Exporting information from SAAM II to a spreadsheet is also illustrated in this tutorial.

It should be pointed out that, while this tutorial will focus on tables created by SAAM II in the **Tables** window, SAAM II generates other tables of output that can be exported to a spreadsheet. For example, the results in the **Statistics** window following a Fit can be exported to a spreadsheet following the same set of rules illustrated in this tutorial for information in a **Tables** window.

Part 1. Exporting data for plotting

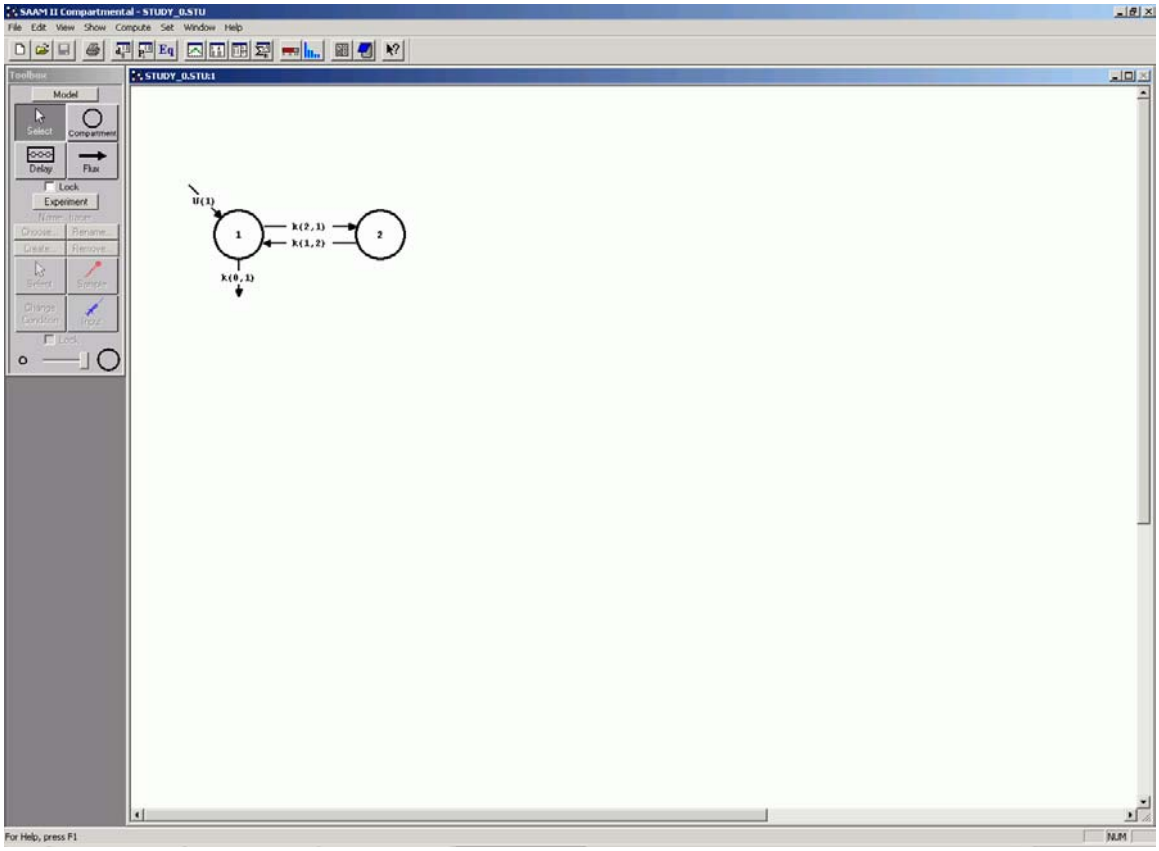
Suppose one desires to provide a customized plot of an associated sample(s) and data. Information to construct a plot can be created in a **Table** following a Solve or Fit and exported to a graphics application. The **Tables** window's controls are similar to the **Plot** window's controls. They are found in the **Set** menu in **Plot/Table Variables** and **Plot/Table Scale**. In **Plot/Table Variables**, you choose the variables you want to appear in your table. In **Plot/Table Scale**, you set the scale (length of time or time interval) of your table.

1. **Start** the **SAAM II Compartmental** application. The **SAAM II Compartmental** main window will open.

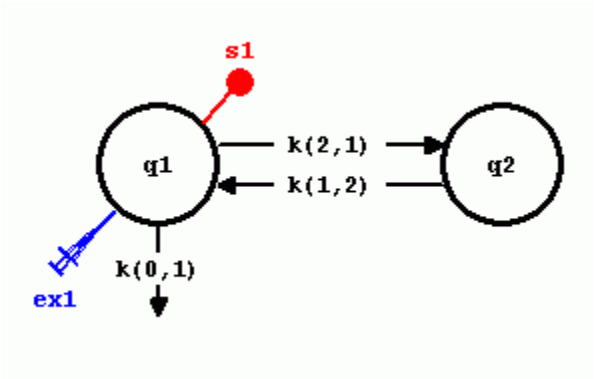
2. Open the **SAAM II Compartmental** study file **study_0**.

   a. In the **File** menu, click **Open**. The file **study_0.stu** should appear in the file list; if it does not, find the folder where you put this tutorial. **Open** the study file.

   b. In the **File** menu, click **Open**. The **SAAM II Compartmental** main window will appear as shown below:



3. View the model and the experiment on the model. In the **SAAM II Toolbox**, click **Experiment**. The model of the experiment will appear on the **Drawing Canvas** as follows:



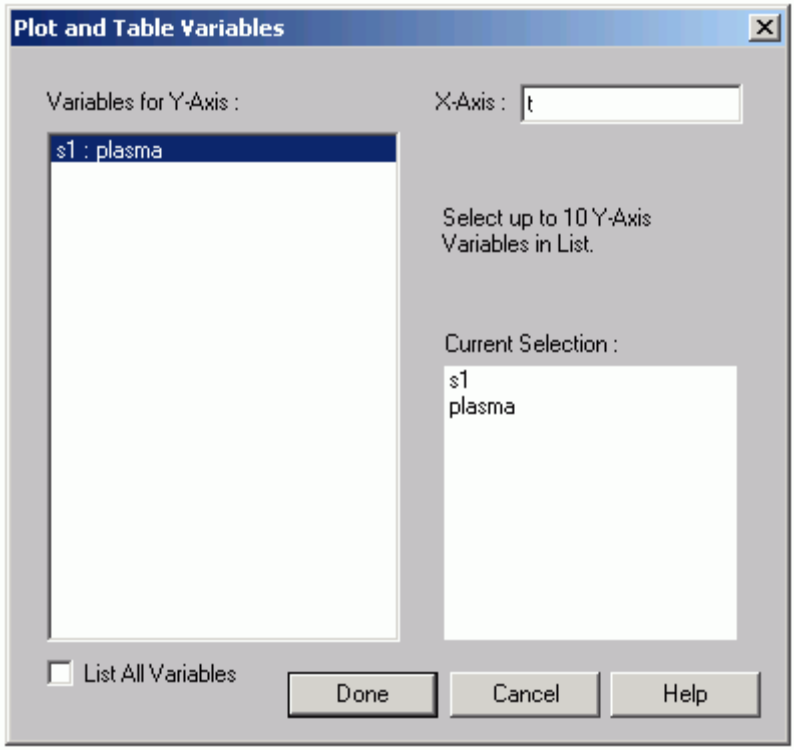
This is the experimental model developed and used in the **Getting Started with Compartmental** tutorial.

4. Solve the model and view the solution.

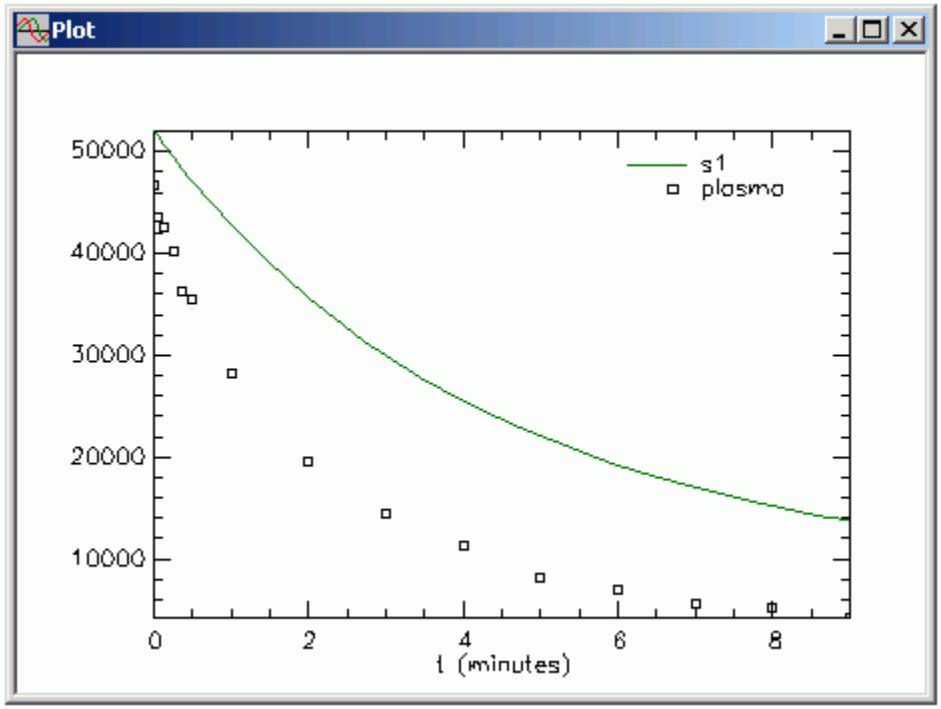
   a. In the **Compute** menu, click **Solve**, or alternatively, on the **SAAM II Toolbar,** click **Solve**  .

   b. In the **Show** menu, click **Plot**, or alternatively, on the **SAAM II Toolbar,** click **Plot**  . The **Plot and Table Variables** dialog box will open. Be sure the **List All Variables** check box is not selected.

   c. Click **s1:plasma** to move this to the **Current Selection** pane. The **Plot and Tables Variables** dialog box will appear as follows:



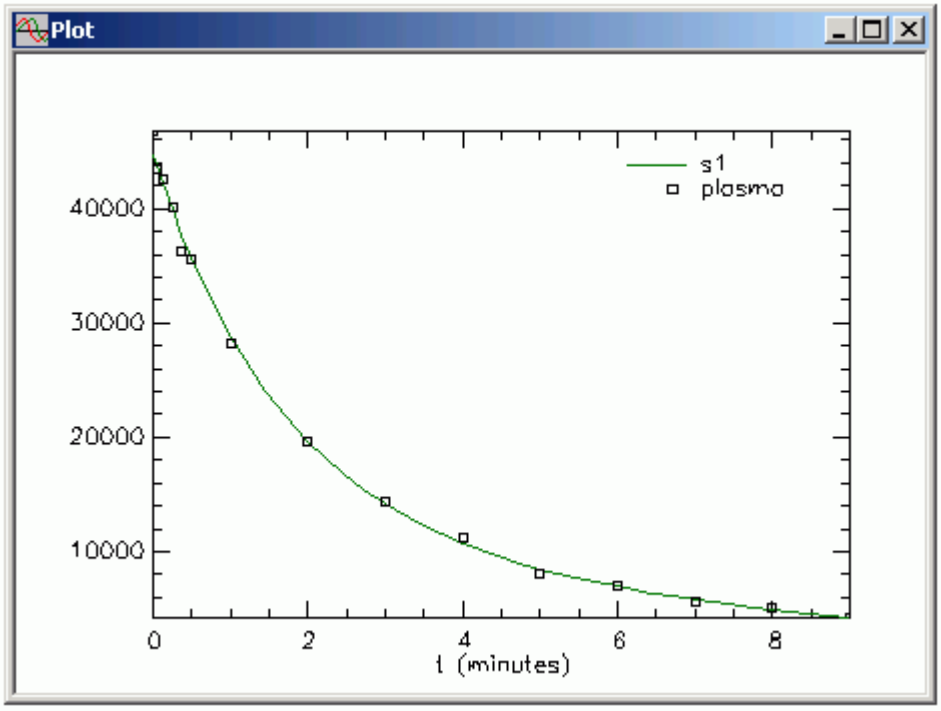
d. Click **Done**. Your plot will appear as shown below (in linear mode):



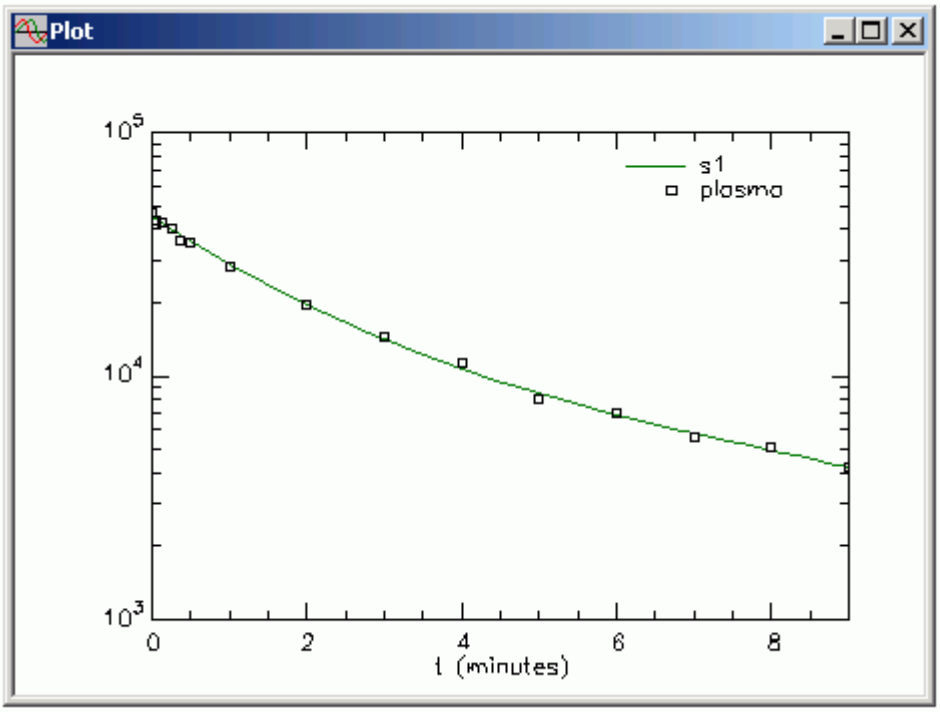
Leave the **Plot** window open.

*Leaving the **Plot** window open*. During your modeling exercise, you can leave the **Plot** window open and perform operations such as changing parameter values, solving and fitting. As soon as you change a characteristic of your model such as changing the value of the parameter, the solution will disappear from your plot. As soon as you Solve or Fit, the updated solution will reappear.

5. Fit the model to your data. In the **Compute** menu, click **Fit**, or alternatively, on the **SAAM II Toolbar** click **Fit**  . Since the **Plot** window was open during the "Fit", the **Plot** window will be updated as shown below:



If you wish to see the plot in semilog mode, in the **View** menu, click **Semilog**. The plot will change from linear to semilog as shown below:



Linear and semilog plots. To switch back and forth between linear and semilog plots, in the **View** menu, locate **Semilog**. If **Semilog** is checked, the plot is semi-logarithmic. If **Semilog** is not checked, the plot is linear. To switch back and forth, you need to go to the **View** menu, and select or cancel the **Semilog** option.

Close the **Plot** window.

6. View the results in tabular form.

   a. In the **Show** menu, click **Table**, or alternatively, on the **SAAM II Toolbar,** click **Table**  . Since the **Plot** window was previously opened with a plot of **s1** and **plasma**, the **Table** window will open as follows:

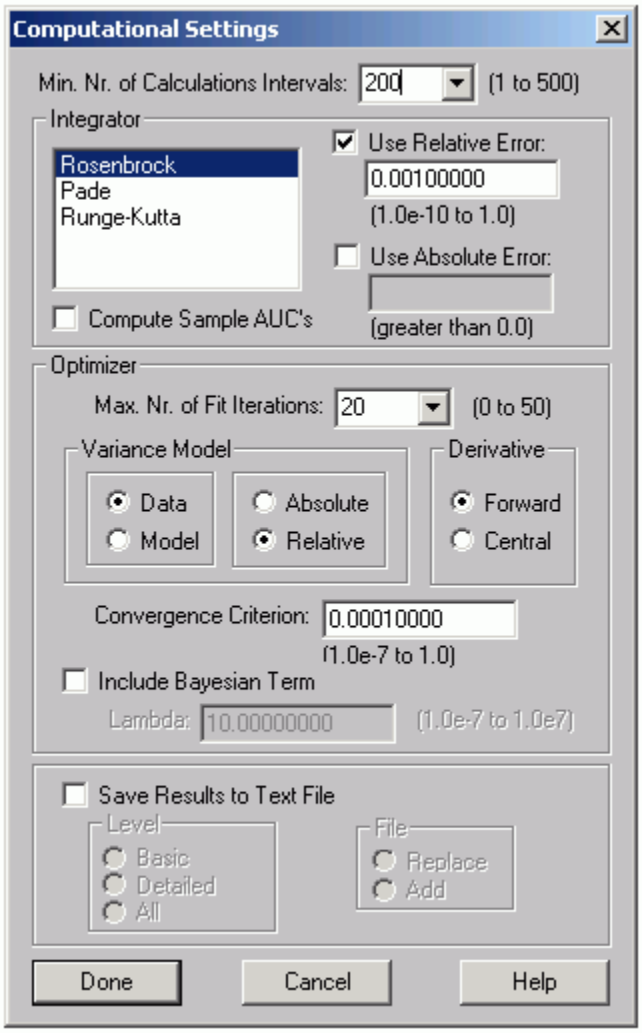
Table

t	sl	plasma
0.000	44754.732	-
7.00000e-003	44608.789	46780.000
4.20000e-002	43887.777	43522.000
0.125	42234.517	42535.000
0.250	39887.687	40125.000
0.375	37701.625	36221.000
0.500	35664.642	35562.000
0.750	31995.409	-
1.000	28802.603	28194.000
1.450	24050.218	-
1.725	21664.652	-
2.000	19601.193	19573.000
2.450	16796.027	-
2.725	15368.982	-
3.000	14121.006	14403.000
3.450	12397.968	-
3.725	11506.245	-
4.000	10715.665	11278.000
4.450	9603.457	-
4.725	9016.183	-
5.000	8487.392	8081.000
5.450	7728.050	-
5.725	7318.556	-
6.000	6944.009	6999.000
6.450	6395.269	-
6.725	6093.436	-
7.000	5813.411	5653.000
7.450	5395.888	-
7.725	5162.366	-
8.000	4943.185	5139.000
8.450	4611.791	-
8.725	4424.042	-
9.000	4246.276	-
9.000	4246.276	4210.000

Generating tables. The table contains the model calculated values at the times at which there are data, and at times at which there are "calculation points". The "calculation points" are determined by the Minimum Number of Calculation Intervals. This is a mechanism in SAAM II by which the user can control the number of values for samples that are saved for plotting and tabular purposes. Some plotting packages may require more sample calculations. This can be achieved by increasing the Minimum Number of Calculation Intervals.

b. In the **Compute** menu, click **Computational Settings**. The **Computational Settings** dialog box will open.

c. Change the **Min. Nr. of Calculation Intervals** from "20" to "200". The **Computational Settings** dialog box will appear as follows:



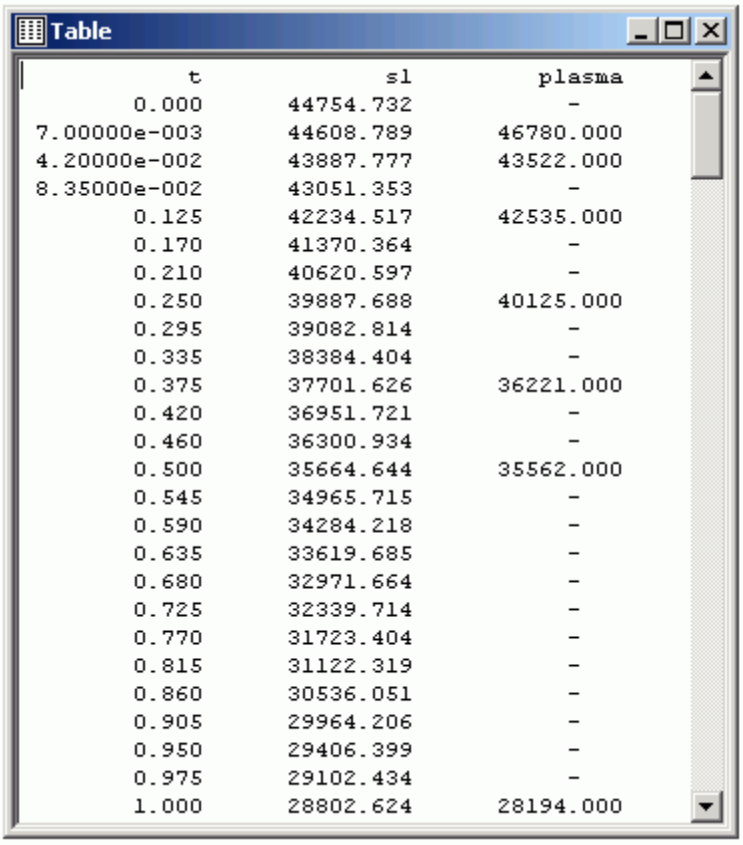
d. Click **Done**. The **Table** window will appear as follows:

Table

t	s1	plasma
7.00000e-003	-	46780.000
4.20000e-002	-	43522.000
0.125	-	42535.000
0.250	-	40125.000
0.375	-	36221.000
0.500	-	35562.000
1.000	-	28194.000
2.000	-	19573.000
3.000	-	14403.000
4.000	-	11278.000
5.000	-	8081.000
6.000	-	6999.000
7.000	-	5653.000
8.000	-	5139.000
9.000	-	4210.000

Changing a computational setting. When you change a computational setting in the **Computational Settings** dialog box, this will change the characteristics of the current solution. In this case, the Minimum Number of Calculation Intervals has been increased. The reason why there are no values for **s1** is that the computational settings have changed. The **Table** window can be updated with a Solve or a Fit.

e. Re-Solve the model. The **Table** window will appear (in part) as follows:



t	s1	plasma
0.000	44754.732	-
7.00000e-003	44608.789	46780.000
4.20000e-002	43887.777	43522.000
8.35000e-002	43051.353	-
0.125	42234.517	42535.000
0.170	41370.364	-
0.210	40620.597	-
0.250	39887.688	40125.000
0.295	39082.814	-
0.335	38384.404	-
0.375	37701.626	36221.000
0.420	36951.721	-
0.460	36300.934	-
0.500	35664.644	35562.000
0.545	34965.715	-
0.590	34284.218	-
0.635	33619.685	-
0.680	32971.664	-
0.725	32339.714	-
0.770	31723.404	-
0.815	31122.319	-
0.860	30536.051	-
0.905	29964.206	-
0.950	29406.399	-
0.975	29102.434	-
1.000	28802.624	28194.000

Now there are many more values for **s1** that have been saved in tabular form. This is because of the increase in the minimum number of calculation intervals.

You can copy and paste the contents of the table into a plotting application. Alternatively, you can copy the contents into a spreadsheet as illustrated below.

Leave the **Table** window open.

7. Export the contents of the **Table** window to an Excel® spreadsheet.

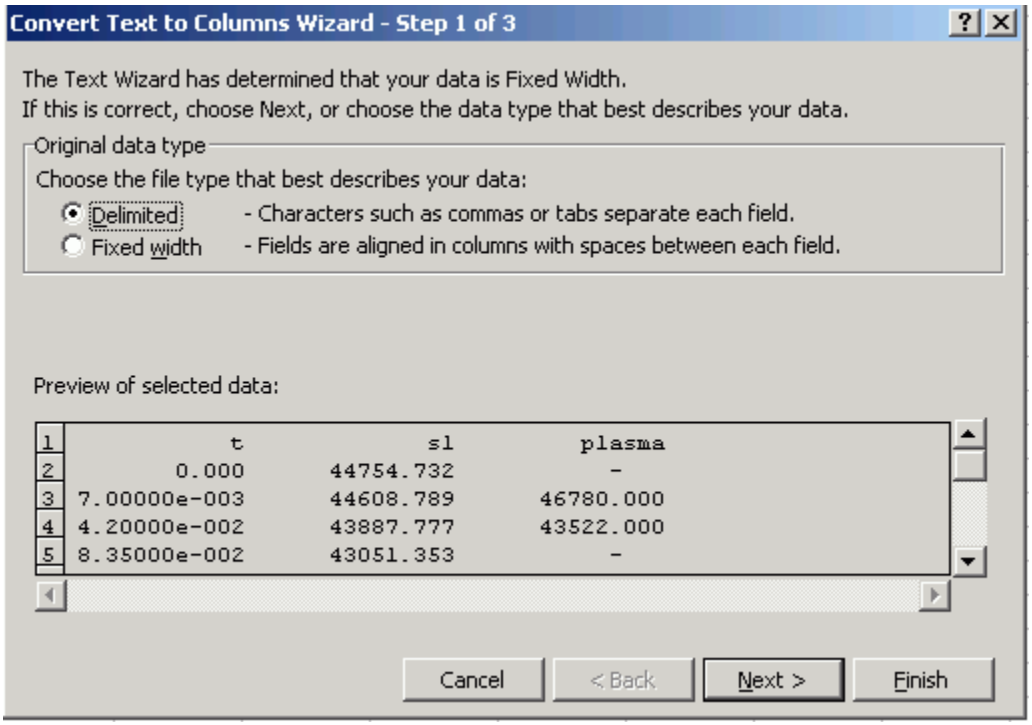
a. Select and copy the information in the **Table** window. In the **Edit** menu click **Select All**. Then, in the **Edit** menu, click **Copy**.

b. Open Excel®.

c. Click the A-1 cell; then on the **Edit** menu, click **Paste**.

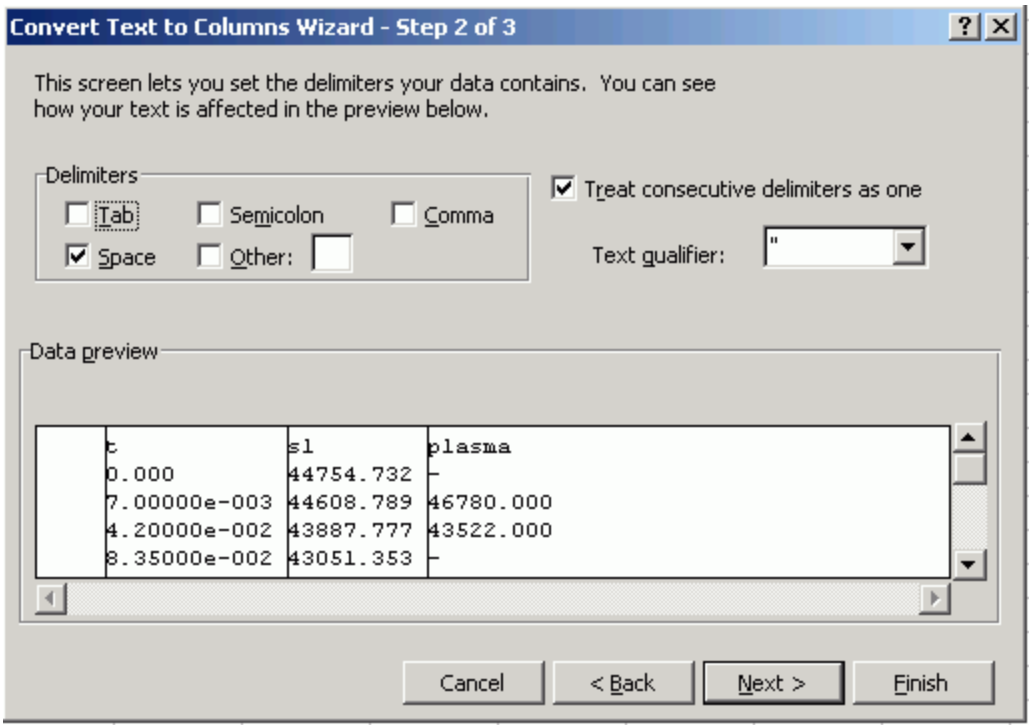
d. On the **Data** menu, click **Text to Columns …**.

e. In the **Original Data Type** pane, select **Delimited**. The **Convert Text to Column Wizard – Step 1 of 3** dialog box will appear as follows:



f. Click **Next**.

g. In the **Delimiters** pane, select **Space**. The **Convert Text to Column Wizard – Step 2 of 3** dialog box will appear as follows:



h. Click **Next**.

i. Click **Finish**. The Excel® spreadsheet will appear in part as follows:

	A	B	C	D
1		t	s1	plasma
2		0	44754.73	-
3		7.00E-03	44608.79	46780
4		4.20E-02	43887.78	43522
5		8.35E-02	43051.35	-
6		0.125	42234.52	42535
7		0.17	41370.36	-
8		0.21	40620.6	-
9		0.25	39887.69	40125
10		0.295	39082.81	-
11		0.335	38384.4	-
12		0.375	37701.63	36221
13		0.42	36951.72	-
14		0.46	36300.93	-
15		0.5	35664.64	35562
16		0.545	34965.72	-
17		0.59	34284.22	-
18		0.635	33619.69	-
19		0.68	32971.66	-
20		0.725	32339.71	-
21		0.77	31723.4	-
22		0.815	31122.32	-
23		0.86	30536.05	-
24		0.905	29964.21	-
25		0.95	29406.4	-
26		0.975	29102.43	-
27		1	28802.62	28194

The data are in columns B, C and D. If you delete column A and left-justify the entries in the other columns, the Excel® spreadsheet will appear in part as follows:

	A	B	C
1	t	s1	plasma
2	0	44754.73	-
3	7.00E-03	44608.79	46780
4	4.20E-02	43887.78	43522
5	8.35E-02	43051.35	-
6	0.125	42234.52	42535
7	0.17	41370.36	-
8	0.21	40620.6	-
9	0.25	39887.69	40125
10	0.295	39082.81	-
11	0.335	38384.4	-
12	0.375	37701.63	36221
13	0.42	36951.72	-
14	0.46	36300.93	-
15	0.5	35664.64	35562
16	0.545	34965.72	-
17	0.59	34284.22	-
18	0.635	33619.69	-
19	0.68	32971.66	-
20	0.725	32339.71	-
21	0.77	31723.4	-
22	0.815	31122.32	-
23	0.86	30536.05	-
24	0.905	29964.21	-
25	0.95	29406.4	-
26	0.975	29102.43	-
27	1	28802.62	28194

j. SAAM II calculates two values at the end of the experiment. If you scroll through the Excel® spreadsheet, you will find two entries for day 9. You can delete the entry at day 9 that does not have the datum associated with it.

You can save the Excel® file if you wish. It has been saved and provided as part of this tutorial as **PlotExcel**.

You can now use this file in Excel® or in other software applications.

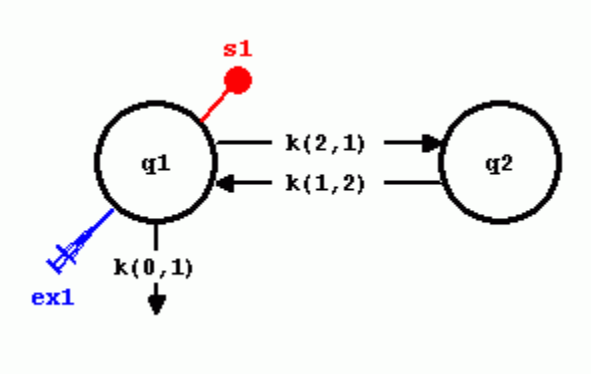
Quit the **SAAM II Compartmental** application. Do not save the changes to **study_0**.

Part 2. Exporting residuals or weighted residuals

Suppose one wants to use a statistical package to test for goodness-of-fit by performing the runs test. Information on the residuals or weighted residuals can be created in a **Table** following a Fit, and exported directly to a statistical application or a spreadsheet. This part of the tutorial will show how to export the weighted residuals to a spreadsheet.

1. **Start** the **SAAM II Compartmental** application and open the **SAAM II Compartmental** study file **study_0**.

2. View the model and the experiment on the model. In the **SAAM II Toolbox**, click **Experiment**. The model of the experiment will appear on the **Drawing Canvas** as follows:



   This is the experimental model developed and used in the **Getting Started with Compartmental** tutorial.

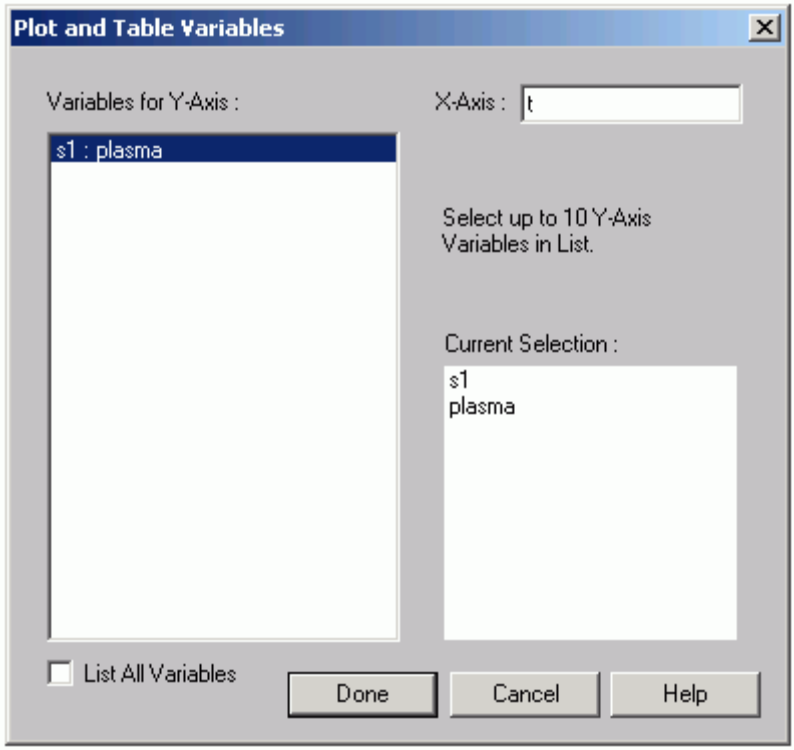
3. Fit the model and view the solution.

   a. In the **Compute** menu, click **Fit**, or alternatively, on the **SAAM II Toolbar** click **Fit**  .

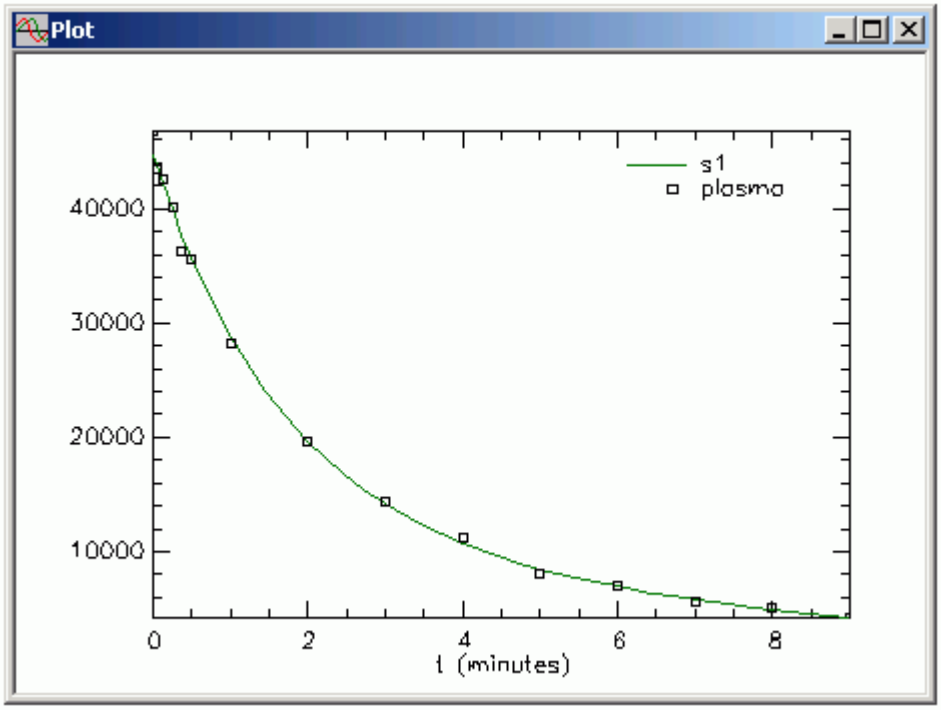
   Fit without a Solve. You can proceed immediately to Fit without first Solving. The reason is that solving in an integral part of the fitting process.

   b. In the **Show** menu, click **Plot**, or alternatively, on the **SAAM II Toolbar,** click **Plot**  . The **Plot and Table Variables** dialog box will open. Be sure the **List All Variables** check box is not selected.

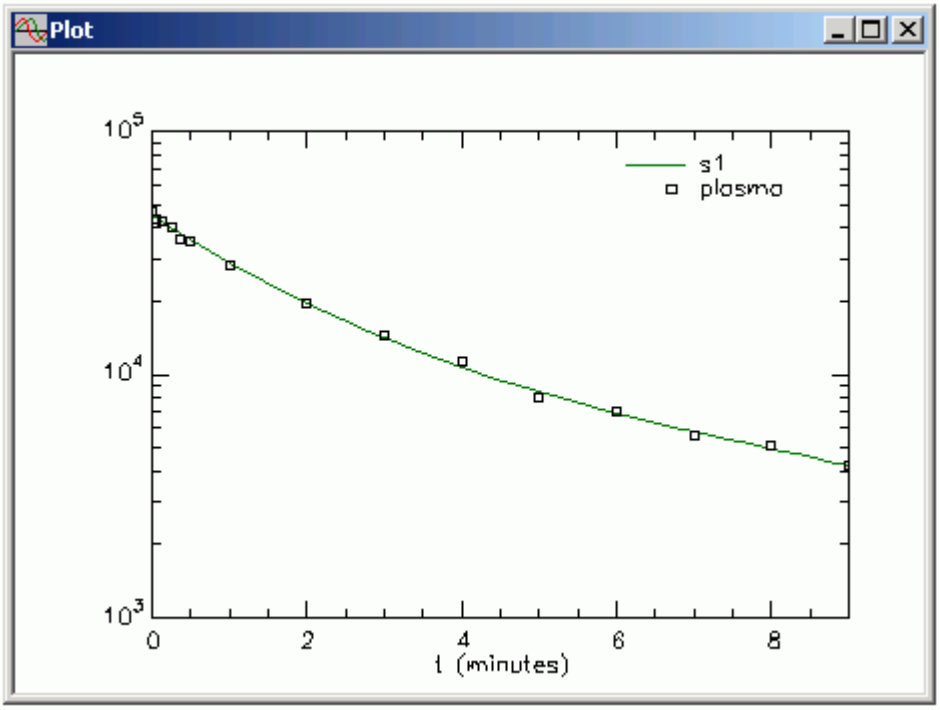
   c. Click **s1:plasma** to move this to the **Current Selection** pane. The **Plot and Tables Variables** dialog box will appear as follows:



d. Click **Done**. Your plot will appear as shown below (in linear mode):



If you wish to see the plot in semilog mode, in the **View** menu, click **Semilog**. The plot will change from linear to semilog as shown below:



Linear and semilog plots. To switch back and forth between linear and semilog plots, in the **View** menu, locate **Semilog**. If **Semilog** is checked, the plot is semi-logarithmic. If **Semilog** is not checked, the plot is linear. To switch back and forth, you need to go to the **View** menu, and select or cancel the **Semilog** option.

Leave the **Plot** window open.

*Leaving the **Plot** window open*. During your modeling exercise, you can leave the **Plot** window open and perform operations such as changing parameter values, solving and fitting. As soon as you change a characteristic of your model such as changing the value of the parameter, the solution will disappear from your plot. As soon as you Solve or Fit, the updated solution will reappear.

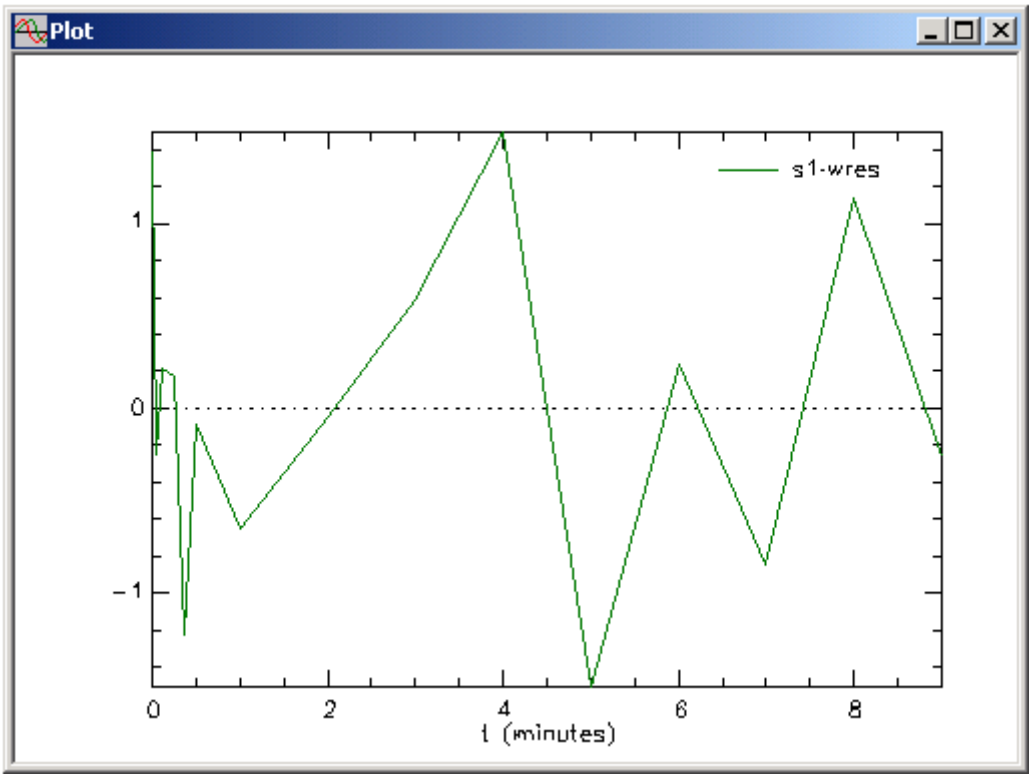
4. View the weighted residuals.

a. In the **Set** menu, click **Plot/Table Variables**. The **Plot and Table Variables** dialog box will open.

b. Check the **List All Variables** check box in the lower left corner of the dialog box.

c. Click **s1_wres** to move this variable to the **Current Selection** pane.

d. Click **Done**. In the **View** menu, click **Semilog** to change the plot to linear mode. The plot of the weighted residuals in linear form will appear as follows:



d. **Close** the **Plot** window.

5. View the results in tabular form.

a. In the **Show** menu, click **Table**, or alternatively, on the **SAAM II Toolbar,** click **Table**  . Since the **Plot** window was open with a plot of **s1_wres**, the **Table** window will open as follows:

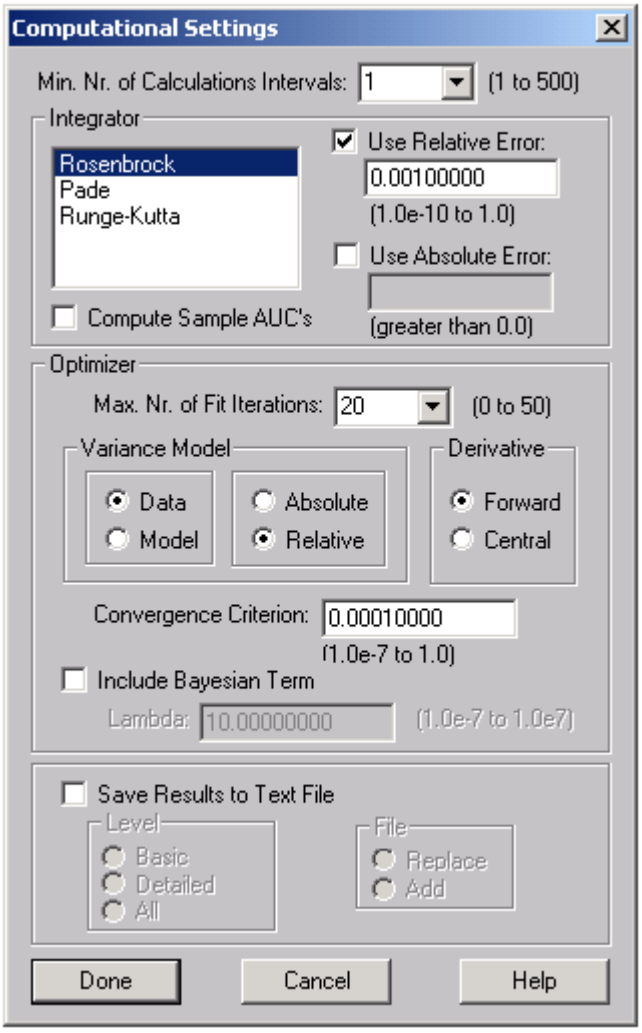
Table

t	sl_wres
0.000	-
7.00000e-003	1.391
4.20000e-002	-2.51860e-001
0.125	0.212
0.250	0.177
0.375	-1.22500e+000
0.500	-8.64952e-002
0.750	-
1.000	-6.46889e-001
1.450	-
1.725	-
2.000	-4.31651e-002
2.450	-
2.725	-
3.000	0.587
3.450	-
3.725	-
4.000	1.494
4.450	-
4.725	-
5.000	-1.50706e+000
5.450	-
5.725	-
6.000	0.235
6.450	-
6.725	-
7.000	-8.50370e-001
7.450	-
7.725	-
8.000	1.142
8.450	-
8.725	-
9.000	-
9.000	-2.58222e-001

Generating tables. The table contains the model calculated values at the times at which there are data, and at times at which there are "calculation points". The "calculation points" are determined by the Minimum Number of Calculation Intervals. This is a mechanism in SAAM II by which the user can control the number of values for samples that can be saved for plotting and tabular purposes. The "runs test" needs calculated values at only the times where there is data. This can be achieved by decreasing the Minimum Number of Calculation Intervals to 1.

b. In the **Compute** menu, click **Computational Settings**. The **Computational Settings** dialog box will open.

c. Change the **Min. Nr. of Calculation Intervals** from "20" to "1". The **Computational Settings** dialog box will appear as follows:



d. Click **Done**. The **Table** window will appear as follows:

Table

t	sl_wres
7.00000e-003	-
4.20000e-002	-
0.125	-
0.250	-
0.375	-
0.500	-
1.000	-
2.000	-
3.000	-
4.000	-
5.000	-
6.000	-
7.000	-
8.000	-
9.000	-

Changing a computational setting. When you change a computational setting in the **Computational Settings** dialog box, this will change the characteristics of the current solution. Note that all the calculated values s1_wres are no longer available as the computational settings have changed. The **Table** window can be updated with a Fit.

e. Re-Fit the model. The **Table** window will appear as follows:

Table

t	sl_wres
0.000	-
7.00000e-003	1.391
4.20000e-002	-2.51800e-001
0.125	0.212
0.250	0.177
0.375	-1.22471e+000
0.500	-8.64747e-002
1.000	-6.46711e-001
2.000	-4.26278e-002
3.000	0.592
4.000	1.502
5.000	-1.49814e+000
6.000	0.243
7.000	-8.44224e-001
8.000	1.146
9.000	-
9.000	-2.54856e-001

This contains the desired residuals except for the zero time point which can be eliminated. SAAM II calculates two values at the final time of the experiment. The duplicate value at day 9 with no residual can also be eliminated.

You can copy and paste the contents of the table into a plotting application. Alternatively, you can copy the contents into a spreadsheet as illustrated below.

Leave the **Table** window open.

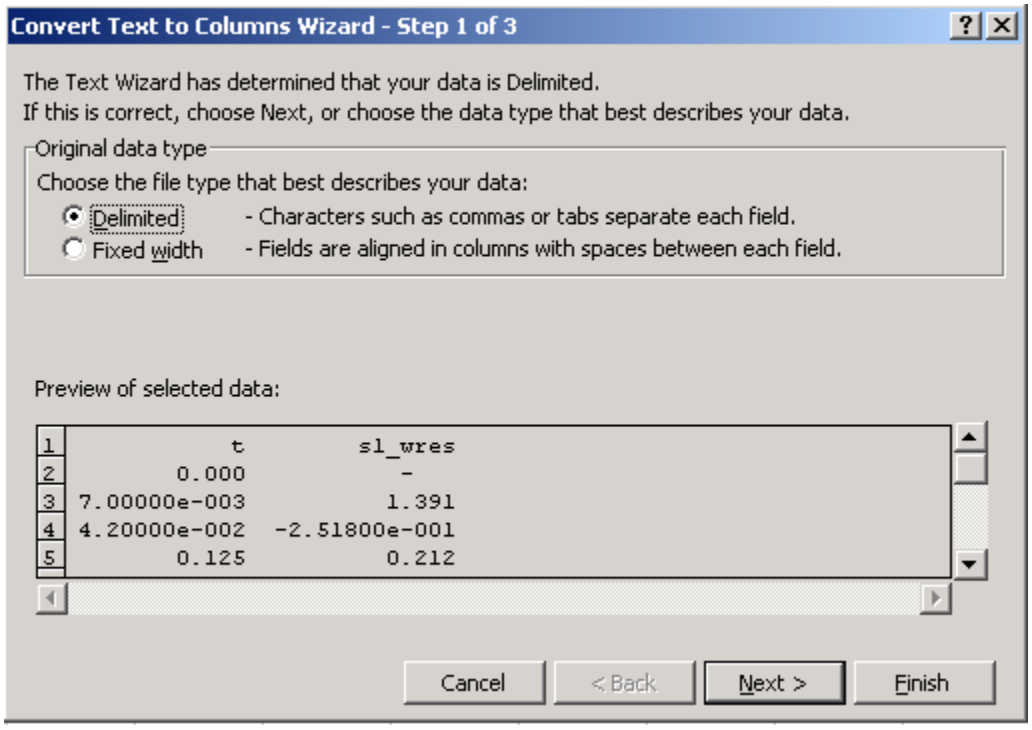
6. Export the contents of the **Table** window to an Excel® spreadsheet.
   a. Select and copy the information in the **Table** window. . In the Edit menu click Select All. Then, in the Edit Menu, click Copy.

   b. Open Excel®.

   c. Click the A-1 cell; then on the **Edit** menu, click **Paste**.

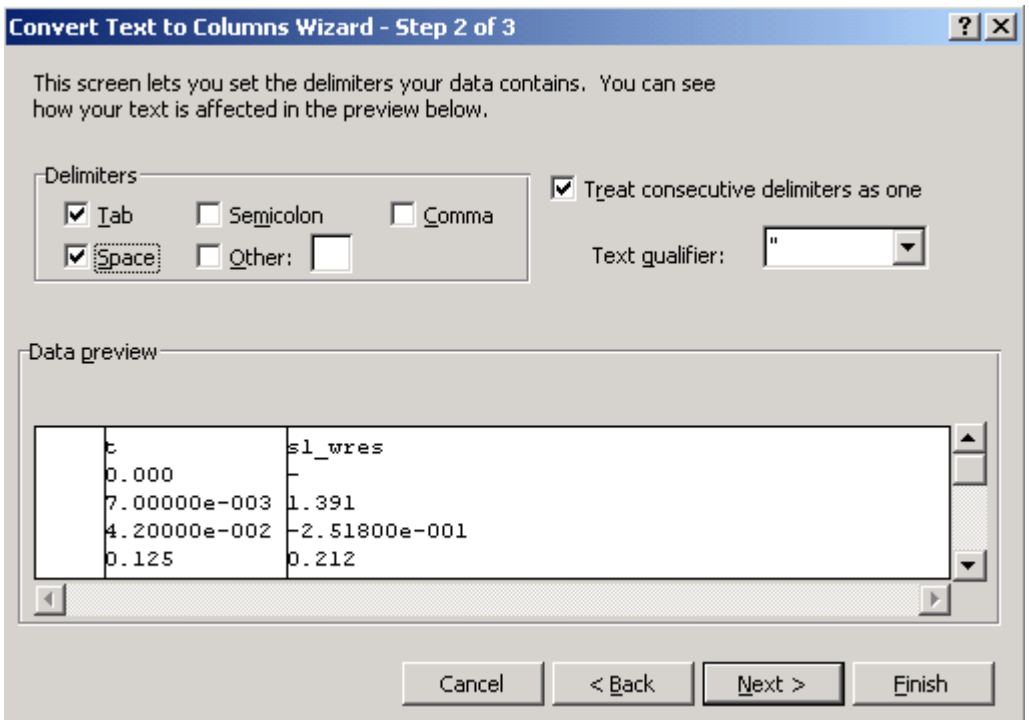
   d. On the **Data** menu, click **Text to Columns …**.

   e. In the **Original Data Type** pane, select **Delimited**. The **Convert Text to Column Wizard – Step 1 of 3** dialog box will appear as follows:



   f. Click **Next**.

g. In the **Delimiters** pane, select **Space**. The **Convert Text to Column Wizard – Step 2 of 3** dialog box will appear as follows:



h. Click **Next**.

i. Click **Finish**. The Excel® spreadsheet will appear in part as follows:

	A	B	C
1		t	s1_wres
2		0	-
3		7.00E-03	1.391
4		4.20E-02	-2.52E-01
5		0.125	0.212
6		0.25	0.177
7		0.375	#########
8		0.5	-8.65E-02
9		1	-6.47E-01
10		2	-4.26E-02
11		3	0.592
12		4	1.502
13		5	##########
14		6	0.243
15		7	-8.44E-01
16		8	1.146
17		9	-
18		9	-2.55E-01

The data are in columns B and C. The "########" are numbers whose format will not fit into the particular cell. When the number format is reset, they will appear.

j. Change the spreadsheet.

(1) Delete column A.

(2) Left-justify the entries in the columns.

(3) Delete the time zero line, and the time 9 line that has no data.

(4) Change the number format to two-decimal places. The Excel® spreadsheet will appear as follows:

	A	B
1	t	s1_wres
2	7.00E-03	1.39
3	4.20E-02	-0.25
4	0.125	0.21
5	0.25	0.18
6	0.375	-1.22
7	0.5	-0.09
8	1	-0.65
9	2	-0.04
10	3	0.59
11	4	1.50
12	5	-1.50
13	6	0.24
14	7	-0.84
15	8	1.15
16	9	-0.25

You can save the Excel® file is you wish. It has been saved and provided as part of this tutorial as **WresExcel**.

You can now use this file in Excel® or in other software applications.

Quit the **SAAM II Compartmental** application. Do not save the changes to **study_0**.

