SAAM II Version 2.2 Basic Tutorials

Working with Plots

	Introduction	Plots – 1
Part 1	Working with line plots	Plots – 3
Part 2	Working with Plot and Table Variables	Plots – 7
Part 3	Working with Plot and Table Scales	Plots – 18
Part 4	Working with Plot and Table Labels	Plots – 30
Part 5	Increasing the resolution of a plot	Plots – 35
Part 6	Changing the X-axis variable	Plots – 42

UPDATE. There might be slight variations in the graphical representations and plot options in the latest version 2.2.3. However, navigating through them should be intuitive, as the core principles remain consistent This page is intentionally left blank

Working with Plots

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 view the results of your modeling exercise using plots. You will learn

- How to view line plots of your data (Part 1)
- How to change plot variables (Part 2)
- How to change the viewing areas of the X- and Y-axis (Part 3)
- How to create labels on your plots (Part 4)
- How to increase the resolution of your plots (Part 5)
- How to change the variable on the X-axis (Part 6)

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** examples.

Remember **study_0** is a study file for an experiment lasting 9 days.

Introduction

This tutorial focuses on the features involved in viewing and refining plot output from SAAM II. The first part will show you have to create line plots of your data, and how creating such plots can help you in the early stages of model development and testing.

The next three parts of the tutorial will discuss the options in the **Set** menu when a **Plot** window is current. In these parts, the independent variable will always be "t" for time. In Part 6 you will learn how to change the variable on the X-axis.

In Part 5 you will learn how to increase the resolution of your plot. This is very useful when your model solution is changing quickly. It is also useful if you wish to export the information about your plot to another plotting package.

This tutorial will not discuss the Quick Plot feature. Quick Plot permits visualizing plots rapidly but, except for switching between linear and semilog, you cannot change the format of the plot. Remember you can obtain a quick plot of any object in your model on the **Drawing Canvas** by clicking on that object, and then in the **View** menu, click **Quick Plot**.

SAAM II is not intended to be a graphics software tool. The intent of the plotting options in SAAM II is to help you in your modeling exercises. For presentation graphics, you can save the results from SAAM II in, for example, a table and use this in your favorite graphics package.

Part 1. Working with line plots

Line plots are a convenient way by which you can learn about characteristics in your data before you start your modeling exercise. Line plots can help you decide how many compartments you may need in your model, and can be used to help obtain initial parameter estimates for your model. Line plots in SAAM II are created by linear extrapolation between sequential pairs of data.

- 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. The file **study_0.stu** should appear in the file list; if it does not, find the folder where you put this tutorial.
 - 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. Create a line plot of the data.
 - a. In the **Show** menu, click **Plot**, or alternatively, on the **SAAM II Toolbar**, click **Plot Image:** The **Plot and Table Variables** dialog box will open. The **List All Variables** check box is not selected so **s1:plasma** is the only option in the **Variables for Y Axis** pane.
 - b. In the **Plot and Table Variables** dialog box, select the **List All Variables** check box. All variables that can be plotted will appear in the **Variables for Y Axis** pane.
 - c. Click **plasma** to add this to the **Current Selection** pane. The **Plot and Table Variables** dialog box will appear as shown below:



d. Click **Done**. A plot of the "plasma" data will appear in the **Plot** window.

e. In the **View** menu, click **Line Plot**. The line plot will appear in linear mode as follows:



f. If you wish, you can view the line plot in semi-log mode. In the **View** menu, click **Semilog**. The line plot will change to a semi-log plot as shown below:





Using line plots. You can see immediately from this line plot that the data do not decay monoexponentially, so the model used to describe them cannot be a one-compartment model. When you are starting a modeling exercise from scratch, it is always a good idea to look at your data using the line plot feature in SAAM II.





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 semilogarithmic. 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.



5. Close the **Plot** window.

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

Part 2. Using the "Plot/Table Variables" command in the "Set" menu.

There are three options available in the **Set** menu when a **Plot** window is open. One allows you to choose the variables to be plotted on the Y- and X-axes. The second allows you to change the scale on the Y- and X-axis. The last allows you to label your plots. This part of the tutorial will show you have to use the **Plot/Table Variables** command in the **Set** menu to change the variable on the Y-axis only. Changing the variable on the X-axis is discussed in Part 6.

A new feature introduced in SAAM II version 2.1 permits you to access these options with new tools on the **SAAM II Toolbar**. The old **Toolbar** is shown below:

<u>15</u> 5	SAAM II Compartmental - CAD.PART1.END.STU									
File	Edit	View	Show	Compute	Set	Window	Help			
D	6		6		Eq			• • • • •	BB 🕘	N ?

The enhanced **Toolbar** is:

i s	SAAM II Compartmental - STUDY_0.STU										
File	Edit	View	Show	Compute	Set	Window	Help				
D	6		9		Eq			• X 10		BB 🖑	\ ?

After the **Fit** tool, there are three new tools that are dimmed. When a **Plot** is open, the **Toolbar** will appear:

i s	🚼 SAAM II Compartmental - HYDROP4.STU										
File	Edit	View	Show	Compute	Set	Window	Help				
D	6		9	$\overline{d_j^{\text{H}}} \; \underset{{I\!\!R}}{\overset{I\!\!H}{=}} \;$	Eq			• × I0		H 🖑	№ ?

The three new tools permit you to rapidly open the **PLOT AND TABLE VARIABLES**, **PLOT AND TABLE SCALE**, and **PLOT LABEL** dialog boxes.



Accessing the options for plots. A second quick method by which you can open the **SET** menu when a **PLOT** is active is to right click on the plot. If you right click inside the plot window, the following menu selection will open, and you can proceed to change Variables, Scale or Labels; you may also use this menu to change the plot to/from Semilog, to/from Linear, turn on the Grid or Line Plot and Copy or Export the plot.

Variables Scale Labels	
Grid Semilog Line Plot Tile Plots	
Copy Export plot	Ctrl+C





Plot and Table Variables. The purpose of the **Plot/Table Variables** command is to allow you to plot any variable in your model against an independent variable. The default independent variable is "t." An example of the Plot and Table Variables dialog box is shown below.

Plot and Table Variables					×
Variables for Y-Axis	x-	-Axis	t		
s1:plasma	s v	Gelect up Variables	to 10 Y-Axis in List.		
	S F	Surrent S s 1 plasma	election :		
List All Variables	Done	Cano	cel	Help	

The dialog box consists of three panes and one check box. The three panes are the **Variables for Y-Axis**, **X-Axis** and **Current Selection**. The check box is **List All Variables**.

The Variables for Y-Axis pane contains all variables which can be plotted against the variable on the X-axis. When the List All Variables check box is not selected, as is the case above, only those variables associated with samples will be available. When the List All Variables check box is selected, an example of which is shown below, all variables that can be plotted are listed.

Plot and Table Variables	×
Variables for Y-Axis	X-Axis t
ex1.bolus ex1.infusion flux(0,1) flux(1,2) flux(2,1) k(0,1) k(1,2) k(2,1) plasma q1 q2 s1 s1_res s1_res s1_wres t vol	Select up to 10 Y-Axis Variables in List. Current Selection : plasma
I List All Variables Done	Cancel Help

The Current Selection pane shows those variables that you have selected to plot.

In the **X-Axis** box, you can change the name of the independent variable from "t" to another variable in the model.

dino Second

- 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. The file **study_0.stu** should appear in the file list; if it does not, find the folder where you put this 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
Che 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:

Plot and Table Variables	X
Variables for Y-Axis	X-Axis t
	Select up to 10 Y-Axis Variables in List.
	Current Selection :
	s1 plasma
List All Variables	Cancel Help

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. When 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 semilogarithmic. 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.

of the second

Leave the **Plot** window open. If you do not leave the **Plot** window open, when you open the **Set** menu, the options in the **Set** menu for plots will not be available.

- 5. Plot **q1** and **q2**, the solution to the differential equations represented by your compartmental model, versus time.
 - a. In the **Set** menu, click **Plot/Table Variables**. The **PLOT AND TABLE VARIABLES** dialog box will open.

Alternatively, click the **Select variables** tool in the **SAAM II Toolbar**:



The PLOT AND TABLE VARIABLES dialog box will open.



Opening the **PLOT AND TABLE VARIABLES** *dialog box.* There are now three ways to open this dialog box. One is from the **Set** menu, one is using the **Select variables** tool in the **SAAM II Toolbar** and the third way is right-clicking in a plot window.



In the **Plot and Table Variables** dialog box, be sure the **List All Variables** check box is selected. Notice **s1** and **plasma** are selected since this was your last plot.

b. Click **q1**, and then press the **CTRL** key, and click **q2**. The variables **q1** and **q2** will move to the **Current Selection** pane as shown below:

Plot and Table Variables	×
Variables for Y-Axis	X-Axis t
ex1.bolus ex1.infusion flux(0,1) flux(1,2) flux(2,1) k(0,1) k(1,2) k(2,1) plasma q1 q2 s1 s1 res	Select up to 10 Y-Axis Variables in List. Current Selection : q1 q2
s1_res s1_wres t vol	Cancel Help

If you had pressed the **CTRL** key and clicked **q1** and **q2**, because **s1** and **plasma** were already selected, **q1** and **q2** would have been added to the **Current Selection** pane. Clicking **q1** first removes **s1** and **plasma** from the **Current Selection** pane.

c. Click **Done**. The plot of **q1** and **q1** in linear mode will appear as follows (if the plot is not in the linear mode, in the **View** menu, click **Semilog**):



d. In the **View** menu, click **Semilog**. The plot will change to semilog as follows:



- e. Close the **Plot** window.
- 7. Plot the weighted residuals from your "Fit."



Residuals and weighted residuals. For each datum, the residual is the difference between the model calculated value and the datum. For this example, it appears as

s1_res. The weighted residual is the residual times the weight assigned to the datum. It appears as **s1_wres**. The residuals or weighted residuals should be randomly distributed above and below zero. Systematic deviations may indicate that your model is not satisfactory. Analyzing the residuals is an important part of *a posteriori* model identifiability.



a. In the Show menu, click Plot, or alternatively, on the SAAM II Toolbar, click Plot
M. Your plot of q1 and q2 will appear in the Plot window.



SAAM II remembers plots. Once you create a plot, SAAM II will remember the plot variable(s) the next time you open the **Plot** window. Thus if you want to change the variable(s) in the **Plot** window, you must have a **Plot** window current and use the **Plot/Table Variables** option in the **Set** menu.



- b. In the **Set** menu, click **Plot/Table Variables**, or alternatively click the **Select variable** tool in the **SAAM II Toolbox**. Be sure the **List All Variables** check box is selected in the **Plot and Table Variables** dialog box.
- c. Click **s1_wres** (these are the weighted residuals from your "Fit") to move this variable to the **Current Selection** pane as shown below:

Plot and Table Variables	×
Variables for Y-Axis	X-Axis t
ex1.bolus ex1.infusion flux(0,1) flux(1,2) flux(2,1) k(0,1) k(1,2) k(2,1) plasma q1 q2 s1 s1 res	Select up to 10 Y-Axis Variables in List. Current Selection : s1_wres
si wres t vol	
I List All Variables □ Done	Cancel Help

d. Click **Done**. The plot of the weighted residuals will appear as follows:





e. In the **View** menu, click **Semilog** (this will return the plot to a linear plot). The plot of the weighted residuals in linear mode will appear as follows:



f. Close the **Plot** window.

You have now explored some of the options to change the variables for the Y-axis. **Quit** the **SAAM II Compartmental** application. Do not save the changes to **study_0**.

Part 3. Using the "Plot/Table Scale" command in the "Set" menu.

There are three options available in the **Set** menu when a **Plot** window is open. One allows you to choose the variables to be plotted on the Y- and X-axes. The second allows you to change the scale on the Y- and X-axis. The last allows you to label your plots. This part of the tutorial will show you have to use the **Plot/Table Scale** command in the **Set** menu

There are three options available in the **Set** menu when a **Plot** window is open. One allows you to choose the variables to be plotted on the Y- and X-axes. The second allows you to change the scale on the Y- and X-axis. The last allows you to label your plots. This part of the tutorial will show you how to change the variable on the Y-axis only. Changing the variable on the X-axis is discussed in Part 6.

A new feature introduced in SAAM II version 2.1 permits you to access these options with new tools on the **SAAM II Toolbar**. The old **Toolbar** is shown below:



The enhanced Toolbar is:

<u>: </u>	AAM	II Con	ıpartm	ental - ST	UDY_	0.STU					
File	Edit	View	Show	Compute	Set	Window	Help				
D	B		9		Eq			Σ	• X 10	III	▶?

After the **Fit** tool, there are three new tools that are dimmed. When a **Plot** is open, the **Toolbar** will appear:

🚼 SAAM II Compartmental - HYDROP4.STU											
File	Edit	View	Show	Compute	Set	Window	Help				
D	6		9	dji Ri	Eq			$\overline{\Sigma_n^{\pm}}$	• × 10	89	₩?

The three new tools permit you to rapidly open the **PLOT AND TABLE VARIABLES**, **PLOT AND TABLE SCALE**, and **PLOT LABEL** dialog boxes.



Plot and Table Scale. The purpose of the **Plot/Table Scale** command is to allow you to change the scale of the Y- or X-axis so you can visualize areas of your plot in more detail. An example of the **Plot and Table Scale** dialog box is shown below:

ot and Table Sc	ale	
-X Avis	Minimum	Maximum
AutoScale	0.0	9.0000000
C Set	0.0	9.0000000
Y Axis		
AutoScale	4210.00000000	52000.00000000
C Set	4210.00000000	52000.00000000

The dialog box consists of two panes, the **X** Axis and **Y** Axis pane. Within both panes are the AutoScale and Set options. The default for both is AutoScale; SAAM II will determine for a particular plot what the most appropriate values for the Minimum and Maximum are.

If you select the **Set** option, then you can enter your own values for the **Minimum** or **Maximum**

0-0

- 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. The file **study_0.stu** should appear in the file list; if it does not, find the folder where you put this 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
 Image: 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. Your plot will appear as shown below (in linear mode):



Leave the **Plot** window open.

5. View details of the solution between time zero and 1.5 days.

It is clear that the model predicted value at time zero is higher than the initial data would suggest. This means that *vol* is not large enough. However, without having a better view of the initial decay, it is difficult to tell how to change *vol*.

a. In the **Set** menu, click **Plot/Table Scale**. Alternatively, click the **Set scales** tool in the **SAAM II Toolbar**:



The Plot and Table Scale dialog box will open as follows:

ot and Table Sca	ale	l i i i i i i i i i i i i i i i i i i i
X Axis	Minimum	Maximum
 AutoScale 	0.0	9.0000000
C Set	0.0	9.0000000
Y Axis		
AutoScale	4210.00000000	52000.00000000
O Set	4210.00000000	52000.00000000



0=0

Autoscaling. SAAM II will automatically set the scales for the X-axis and Y-axis based upon the data/solution and the time of the experiment. The default is the **AutoScale** option.

- b. In the **X** Axis pane, choose Set. Type "-0.05" in the Minimum box, and "1.5" in the Maximum box. Setting the minimum equal to -0.05 will allow you to visualize the time zero situation better.
- c. In the **Y** Axis pane, choose Set. Type "30000" in the Minimum box, and "60000" in the Maximum box. The Plot and Table Scale dialog box should appear as shown below:

X Axis	Minimum	Maximum
C AutoScale	0.0	9.0000000
Set	-0.05	1.5
Avie		
C AutoScale	4210.00000000	52000.00000000
C	30000	60000

d. Click **Done**. The plot of the initial decay will appear as follows:



e. Change the estimate for vol.

You can see from the detailed plot that the model predicted concentration value at time zero is about 52,000 while the data would suggest a value closer to 48,000. If you open the **Parameters** dialog box, you will see the initial estimate for *vol* is 2000. The estimate of 52,000 comes from the *dose*, 1.04e+08, divided by the estimated value of 2000 for *vol*. To get closer to the desired 48,000, *vol* must equal 1.04e+08/48000, or approximately 2167.

In the **Parameters** dialog box, change the **Value** for *vol* to 2167. Re-Solve the model. The plot of the initial decay will update as follows:



- f. Close the **Plot** window.
- 6. Fit the model to the data and view the results.
 - a. In the **Compute** menu, click **Fit**, or alternatively, on the **SAAM II Toolbar** click **Fit**
 - b. In the Show menu, click Plot, or alternatively, on the SAAM II Toolbar, click Plot
 M. The plot of the initial decay will appear as follows:





SAAM II remembers plots and scales. Once you create a plot and set the scale of the plot, SAAM II will remember the plot variable(s) and scale the next time you open the **Plot** window. Thus if you want to change the variable(s) and/or scale in the **Plot** window, you must use the **Plot/Table Variables** and/or **Plot/Table Scale** options in the **Set** menu, or the respective tools in the **SAAM II Toolbar**.



- c. In the **Set** menu, click **Plot/Table Scale**, or click the **Set scales** tool in the **SAAM II Toolbar**. The **Plot and Table Scale** dialog box will open.
- d. In both the **X Axis** and **Y Axis** panes, select **Autoscale**. The **Plot and Table Scale** dialog box will appear as follows:

(Axis	Minimum	Maximum
AutoScale	0.0	9.00000000
C Set	-0.05000000	1.5000000
Axis		
AutoScale	4210.00000000	46780.0000000
-	20000 00000000	50000 0000000

e. Click **Done**. The plot will appear (in semilog mode) as follows:



- f. View the final decay in more detail.
 - In the Set menu, click Plot/Table Scale, or click the Set scales tool in the SAAM II Toolbar, or right-click in the plot window and select Scale... The Plot and Table Scale dialog box will open.
 - (2) Set the **Minimum** and **Maximum** in the **X Axis** pane equal to "4.9" and "9.5" respectively. Set the **Minimum** and **Maximum** in the **Y Axis** pane equal to "4000" and "10000" respectively. The **Plot and Table Scale** dialog box will appear as follows:

(Axis	Minimum	Maximum
C AutoScale	0.0	9.0000000
Set	4.9	9.5
C AutoScale	4210.00000000	46780.0000000
~	4000	10000

(3) Click **Done**. The plot of the final decay will appear as follows:



You can see that the model fit of the final decay is quite reasonable, and that the residuals or weighted residuals should be randomly distributed around zero.

- (4) Close the **Plot** window.
- 7. View the weighted residuals.
 - a. In the Show menu, click Plot, or alternatively, on the SAAM II Toolbar, click Plot
 M. Your previous plot will open.
 - b. In the **Set** menu, click **Plot/Table Variables**, or click the **Select variables** tool in the **SAAM II Toolbar**. Be sure the **List All Variables** check box is selected. Notice that **plasma** and **s1** are in the **Current Selection** pane.

- c. Click s1_wres to move this to the Current Selection pane.
- d. Click Done. The plot of the weighted residuals will appear as follows





SAAM II remembers scales. Once you create a plot and set the scale, **SAAM II** will remember the scale the next time you open the **Plot** window. Thus if you want to change the scale in the **Plot** window, you must use the **Plot/Table Scales** option in the **Set** menu, or the **Set scales** tool in the **SAAM II Toolbar**.



- e. In the **Set** menu, click **Plot/Table Scale**, or click the **Set scales** tool in the **SAAM II Toolbar**. The **Plot and Table Scale** dialog box will open.
- f. In the X Axis pane, click Autoscale. In the Y Axis pane, set the Minimum and Maximum values equal to "-2" and "2" respectively. The Plot and Table Scale dialog box will appear as follows:

ot and Table Sca	le	
-X Avis	Minimum	Maximum
AutoScale	0.0	9.0000000
C Set	4.9000000	9.5000000
C AutoScale	-1.50664474	1.49426270
• Set]-2	12
Set	-2	2
Done	Cancel	Help

g. Click Done. The plot of the weighted residuals will appear as follows:



The problem now is that the plot is semilog, and to visualize the weighted residuals, the plot must be linear.

h. In the **View** menu or right-click in the plot window, click **Semilog**. The plot of the weighted residuals will appear as follows:



You can see the weighted residuals are randomly distributed about zero. It is difficult to visualize the initial residuals. You can set the time scale from "0" to "1.5" or "2.0" if you wish to see the initial residuals better. An example is shown below:



i. Close the **Plot** window.

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

Part 4. Using the "Plot/Table Label" command in the "Set" menu.

It is sometimes useful to label plots. In what follows, labels will be put on the plot of **s1** and **plasma**.



Plot and Table Labels. The **Plot/Table Labels** command or **Edit plot labels** tool allows you to put labels on your plots, and to change the font size of the label if you wish. An example of the **Plot Labels** dialog box is shown below:

Plot Labels	×
Title:	
X Axis: t (days)	
Y Axis:	
	Font Size: 7
Done	Cancel Help

There are three boxes in which you can enter information, and the ability to change the font size. The **Title** will appear across the top of your plot. The entries in the **X Axis** and **Y Axis** boxes will appear respectively along the X- and Y-axes.

- 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. The file **study_0.stu** should appear in the file list; if it does not, find the folder where you put this tutorial.
 - 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
M. 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. Your plot will appear as shown below (in linear mode):



Leave the **Plot** window open.

- 4. Fit the model to the data and view the results.
 - a. In the **Compute** menu, click **Fit**, or alternatively, on the **SAAM II Toolbar** click **Fit**. In the plot will be updated as follows:



- 6. Label the plot.
 - a. In the **Set** menu, click **Plot Labels**. Alternatively, click the **Edit plot labels** tool in the **SAAM II Toolbox**, or right-click in the plot window and select Labels.

h	
	<u>v</u>
	Edit plot labels

The **Plot Labels** dialog box will open a shown below:

Plot Labels		×
Title:		
X Axis: t (days)		
Y Axis:		
	Font Size: 7	•
Done	Cancel Help	

- b. Enter the following:
 - (1) In the **Title** box, type "Plasma Decay".
 - (2) In the **X** Axis box, replace "t(days)" with "Days"

(3) In the **Y** Axis box, type "Concentration (dpm/ml)". The **Plot Labels** dialog box will appear as follows:

Plot Labe	ls X
Title:	Plasma Decay
X Axis:	Days
Y Axis:	Concentration (dpm/ml)
	Font Size: 7
Dor	ne Cancel Help

(4) Click **Done**. Your plot will appear as follows:



c. Close the **Plot** window.

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

Part 5. Increasing the plot resolution.

It is sometimes useful to increase the resolution of the plots produced by SAAM II. This is done by increasing the number of Calculations Intervals. As explained below, the Calculations Intervals are used to determine at which time points SAAM II saves solutions for the purpose of creating plots and tables.



Calculation Intervals. For each model experiment, there are a number of calculation points (times) when SAAM II stores the solution to your model for plotting and tabular purposes. The number of calculation points (times) is determined by the number of independent variable data points in the data file and the value of the Minimum Number of Calculations Intervals. The default value for the minimum number of calculation intervals is 20; this value can range from 1 to 500.

There may be times when you wish to increase, or decrease, the resolution of your plot. This happens most frequently when your solution is changing rapidly with, for example, rapid rises and falls in the data. The default value for the minimum number of calculations intervals may not be large enough to permit viewing these details. To view these details effectively, you must increase the minimum number of calculations intervals.

To set this number, in the **Compute** menu, click **Settings**. Enter the desired number in the **Min. Nr. of Calculations Intervals** box at the top of the **Computational Settings** dialog box. Increasing the number of Calculation Intervals results in longer computation times. This won't be noticeable unless you have a complex problem requiring several seconds or minutes to solve.

- ø.
 - 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. The file **study_0.stu** should appear in the file list; if it does not, find the folder where you put this file.
 - b. In the **File** menu, click **Open**. The **SAAM II Compartmental** main window will appear as shown below:

SAAM II Compartmental - STUDY_0.STU	<u> </u>
File Edit View Show Compute Set Window Help	
Toolbox II STUDY_0.STU:1	
Model Select Compartment Delay Flux Lock Experiment	^
Name: tracer k (2,1) 2 Create Remove k (1,2) 2 Select Sample k (0,1)	1
Change Condition Input	•

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
 Che 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. Your plot will appear as shown below (in linear mode):



Leave the **Plot** window open.

- 5. Fit the model to the data and view the results.



6. Increase the resolution of the plot.

a. In the **Compute** menu, click **Settings**. The **Computational Settings** dialog box will open as shown below (notice the **Plot** window is also open but is not available as the **Computational Settings** dialog box is current.)



b. In the **Min. Nr. of Calculations Intervals** box, type 200, or select 200 in the **Min. Nr. of Calculations Intervals** box. The **Computational Settings** dialog box will appear as follows:

Computational Settings
Min. Nr. of Calculations Intervals: 200 💌 (1 to 500)
Integrator Use Relative Error:
Pade Runge-Kutta (1.0e-10 to 1.0)
Use Absolute Error:
Compute Sample AUC's (greater than 0.0)
Optimizer Max. Nr. of Fit Iterations: 20 🔽 (0 to 50)
Variance Model Derivative
Data O Absolute Forward
O Model O Relative O Central
Convergence Criterion: 0.00010000
(1.0e-7 to 1.0)
Lambda: 10.00000000 (1.0e-7 to 1.0e7)
Save Results to Text File Level Basic Replace
C Detailed C All
Done Cancel Help

- c. Click **Done**. The **Computational Settings** dialog box will close. Your plot remains, but the solution disappears. This is because the current solution settings do not match the ones used to create the previous plot.
- 7. Solve your model. The new solution with 200 calculation intervals appears in the **Plot** window. It is not substantially different from the previous plot.



When to increase plot resolution. SAAM II uses the Calculation Intervals to determine when to save solutions for plotting and tabular purposes. Plots are created by linearly interpolating between saved pairs of calculation points. When your solution is rising and falling rapidly as in the case of oral absorption or in calculating 24 hour urine collections, peak values may be missed if the Minimum Number of Calculation Intervals is not large enough. You can often see this in your model solution. When this happens, simply increase the number of intervals.

Consider the following example of a drug which was infused into plasma over a five minute interval. The plot shown as follows is with the default value of 20 for the Minimum Number of Calculation Intervals.



If the minimum is set to 200, the plot will change as follows:



Now you can see the rising portion of the solution.

The default value of 20 for the Minimum Number of Calculation Intervals was determined to be the most efficient in most cases where efficiency relates both to numerical calculation time and the quality of the plot. As with most default settings, it is not perfect and on occasion must be adjusted.

0-0





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

Part 6. Changing the variable on the X-axis.

It is sometimes important to be able to change the variable on the X-axis. In what follows, the variables q2 and q2/q1 will be plotted as a function of the variable q1.



Plot and Table Variables. The **Plot/Table Variables** command allows you to plot any variable in your model against the independent variable "t." In addition, and as will be explained below, in the X-axis box, you can change the name of the independent variable from "t" to another variable in the model. While this situation does not arise often in multicompartmental modeling, it does arise when using the **SAAM II Numerical** application's Michaelis-Menten and Scatchard equations. Here one wants to recreate, for example, the Lineweaver-Burke plot. This involves changing the variable for the X-axis.



- 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. The file **study_0.stu** should appear in the file list; if it does not, find the folder where you put this 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
 Image: 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. Your plot will appear as shown below (in semilog mode):



Leave the **Plot** window open.

- 5. Fit the model to the data and view the results.
 - a. In the **Compute** menu, click **Fit**, or alternatively, on the **SAAM II Toolbar** click **Fit**. The plot will be updated as follows:



Leave the **Plot** window open.

- 6. Plot q2 versus q1.
 - a. In the **Set** menu, click **Plot/Table Variables**, or alternatively click the **Select variables** tool in the **SAAM II Toolbox** or right-click in the plot window. The **Plot and Table Variables** dialog box will open.
 - b. Select the List All Variables check box.
 - c. Click **q2** to move it to the **Current Selection** pane.
 - d. Type "q1" in the **X** Axis box. The **Plot and Table Variables** dialog box will appear as follows:

ot and Table Variables	2
Variables for Y-Axis	X-Axis q1
ex1.bolus ex1.infusion flux(0,1) flux(1,2) flux(2,1) k(0,1) k(1,2) k(2,1) plasma	Select up to 10 Y-Axis Variables in List. Current Selection :
q1 g2 s1 s1_res s1_wres t t vol	q2
I List All Variables	Done Cancel Help

e. Click **Done**. The plot of **q2** versus **q1** will appear in linear mode as follows:



- f. Close the **Plot** window.
- 7. Plot **q2/q1** versus **q1**.
 - a. In the SAAM II Toolbox, click Sample.

- b. Click Compartment **q1** and then click the **Drawing Canvas**. The sample **s2** will appear associated with Compartment **q1**.
- c. Double-click **s2** to open the **Samples Attributes** dialog box. Edit the sample equation to read "s2 = q2/q1". The **Sample Attributes** dialog box will appear as follows:

Sample Attributes	x
Name: s2	
Units:	
Associate with Data Name:	
Equations:	
s2 = q2/q1	3
<u> </u>	
Done Cancel Help	

d. Click **Done**. Your model will appear as shown below:



Notice s2 is connected to both Compartments q1 and q2; this is because both q1 and q2 appear in the sample equation s2. Notice also s2 is open since it is not associated with data.

- e. Re-Solve or Re-Fit the model. Since you have previously "Fitted" the model to the data, both will produce the same result.
- f. In the Show menu, click Plot, or alternatively, on the SAAM II Toolbar, click Plot
 M. The Plot and Table Variables dialog box will open. Be sure the List All Variables check box is selected.



Remembering plots. In general, when you create a plot, the **Plot** window will open with the previous plot. In this way, SAAM II remembers plots. This is not the case in this situation because the previous plot did not have the variable "t" in the **X** Axis box. Because of this, when you open the plot, the **Plot and Table Variables** dialog box opened.



- g. Click s2 to move this variable to the Current Selection pane. Remember s2 is your quotient q2/q1.
- h. Type "q1" in the **X** Axis box. The **Plot and Table Variables** dialog box will appear as follows:

Plot and Table Variables	×
Variables for Y-Axis	X-Axis q1
ex1.bolus ex1.infusion flux(0,1) flux(1,2) flux(2,1) k(0,1) k(1,2) k(2,1) plasma q1 q2 s1 s1_res s1_wres s2 t vol	Select up to 10 Y-Axis Variables in List. Current Selection : s2
List All Variables	e Cancel Help

i. Click **Done**. The plot of **q2/q1** versus **q1** will appear in linear mode as follows:



j. Close the **Plot** window.

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