

Getting Started with Compartmental Tutorial

- Using SAAM II Compartmental
- How to view solutions
- How to build a model
- How to create an experiment
- How to enter data
- How to enter model parameters

Getting Started with SAAM II Compartmental

Prerequisites

This tutorial has no prerequisites. It assumes you know the basics of the Windows operating system. It also assumes you have **SAAM II's Compartmental** application installed on your computer, and that you know how to open the application.

What you will learn in this tutorial

The basic operations of the **SAAM II Compartmental** application:

- How to use a **SAAM II Compartmental** study file.
- How to use **SAAM II Compartmental** computational features.
- How to view solutions.
- How to build a model using the model building tools.
- How to create an experiment on the model using the experiment tools.
- How to enter data, and associate data with samples
- How to enter your model parameters.

Files Required

Study Files: The study file for the **Compartmental** application 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.

Data File: The data file for this tutorial is

study_0.dat

The data file is a text file. (This file is the same as **study_0.dat** that is installed in the **SAAM II** program folder, and referred to in the **SAAM II** User Guide.)

Introduction

This tutorial will show you how to perform the basic operations in the **SAAM II Compartmental** application. It is intended to help the new user get started quickly with **SAAM II**.

This tutorial is divided into two parts. In the first part, you will load an existing SAAM II file. The purpose is to familiarize you with the basic computational operations, and how to view information from solutions. In the second part, you will build a model. This will familiarize you with the tools used to build models and create experiments.

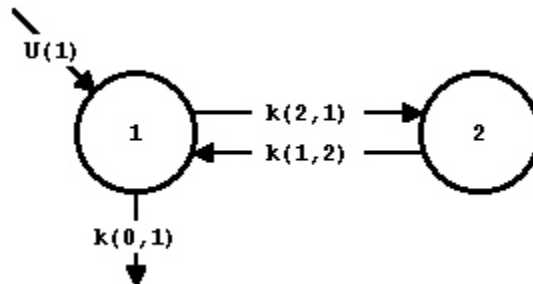


In this SAAM II tutorial, special information or notes to assist the user in using the **Compartmental** application are preceded by the **Compartmental** symbol on the left and end with the small **Compartmental** symbol.



Part 1. Using a Compartmental Study File

This part of the tutorial will show the key components of the model of a system and an experiment on the system, and the fundamental operations of SAAM II - solving, fitting, and viewing solution. You will work with the following two-compartment model.



Transfer coefficients. The SAAM II convention for the transfer coefficients $k(i,j)$ is $k(\text{to},\text{from})$. Thus $k(2,1)$ is the transfer rate to Compartment 2 from Compartment 1. The transfer rate $k(0,1)$ is the rate of irreversible loss from Compartment 1. The input arrow $U(1)$ is for system experiments in tracer-tracee experiments; this will not be discussed in the tutorial.

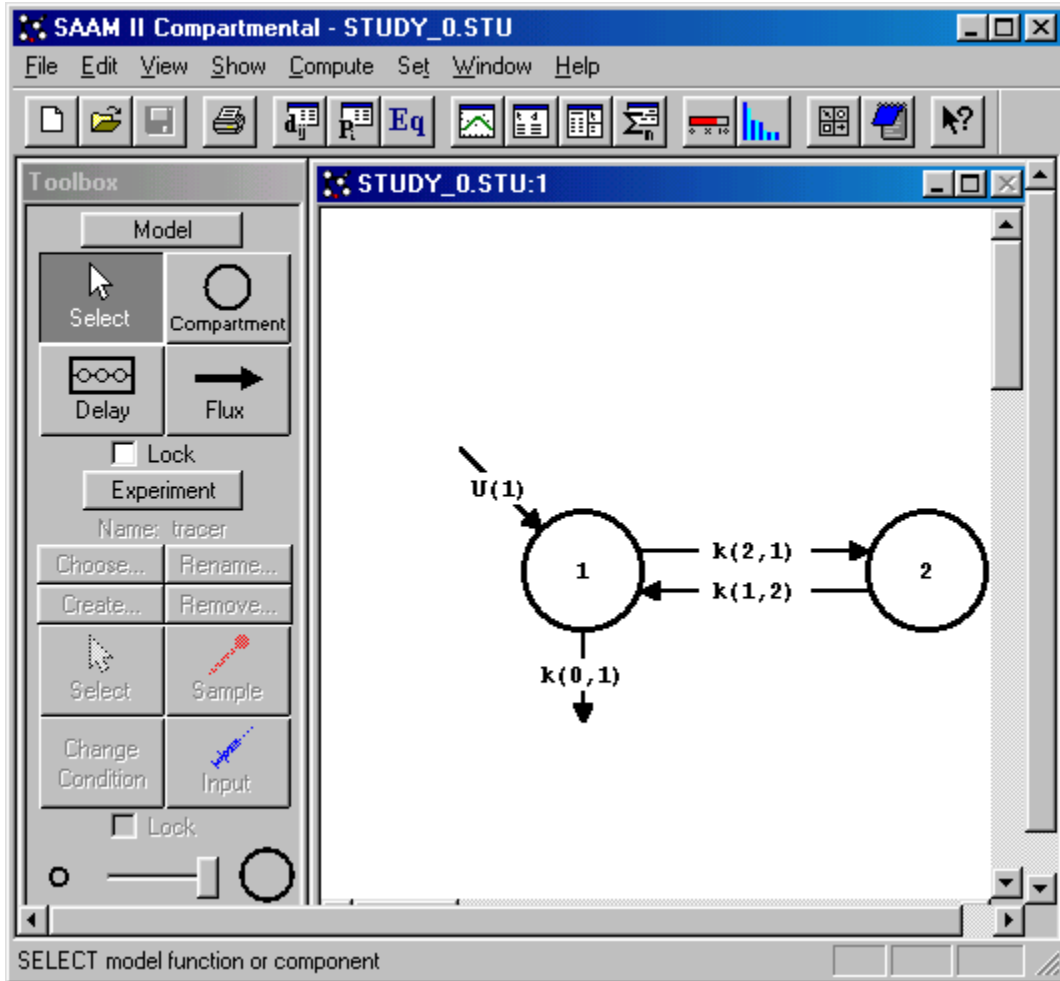


1. Start the SAAM II Compartmental application.
2. Open the SAAM II Compartmental study file **study_0.stu**.

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

In the **File** menu, click **Open**.

The SAAM II Compartmental main window will open as shown below:



The model shown on the **Drawing Canvas** is the SAAM II Compartmental representation of a two-compartment model. In SAAM II terminology, it is called the **System Model**; it is a mathematical representation of how the system functions, and is normally used to interpret tracee data in a tracer-tracee experiment. The input arrow $U(1)$ represents tracee input in a tracer-tracee experiment and will not be discussed in this tutorial.

The SAAM II Compartmental main window consists of four main areas:

The **Menu** bar:

File Edit View Show Compute Set Window Help

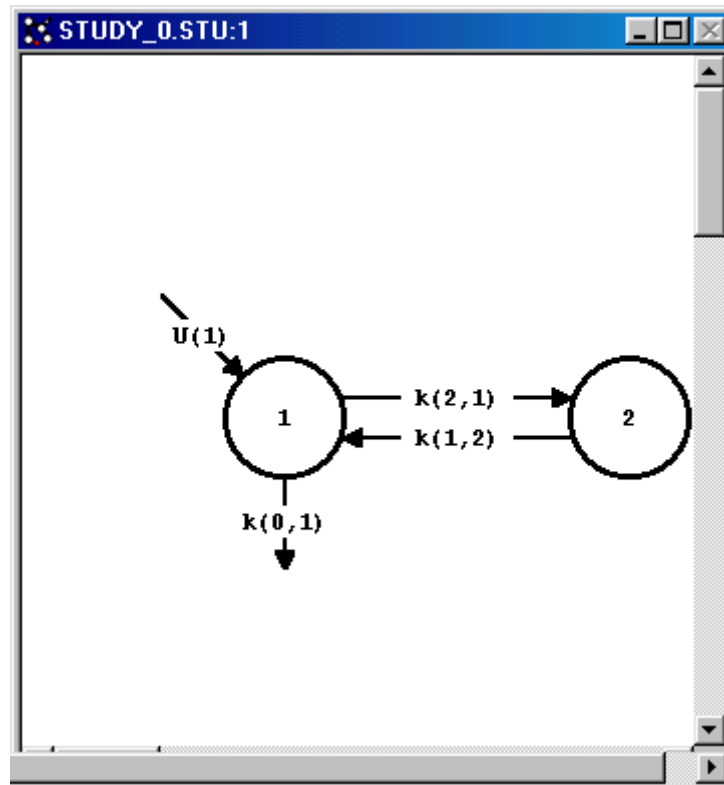
This menu bar contains the SAAM II menu items.

Below the **Menu** bar is the SAAM II **Toolbar**:



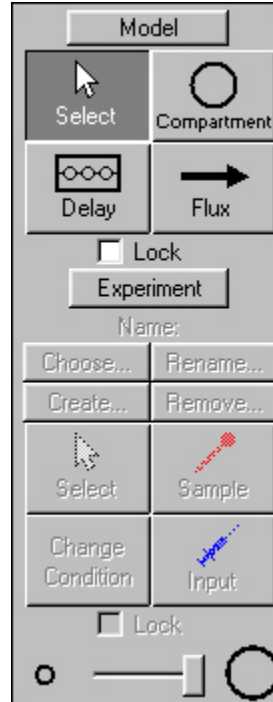
This toolbar contains **SAAM II** specific tools such as “Solve” or “Fit.” Most of the toolbar functions can be found in the **Show** and **Compute** menus.

The **Drawing Canvas** will appear in part as follows:



The **Drawing Canvas** contains the area for building models and creating experiments.

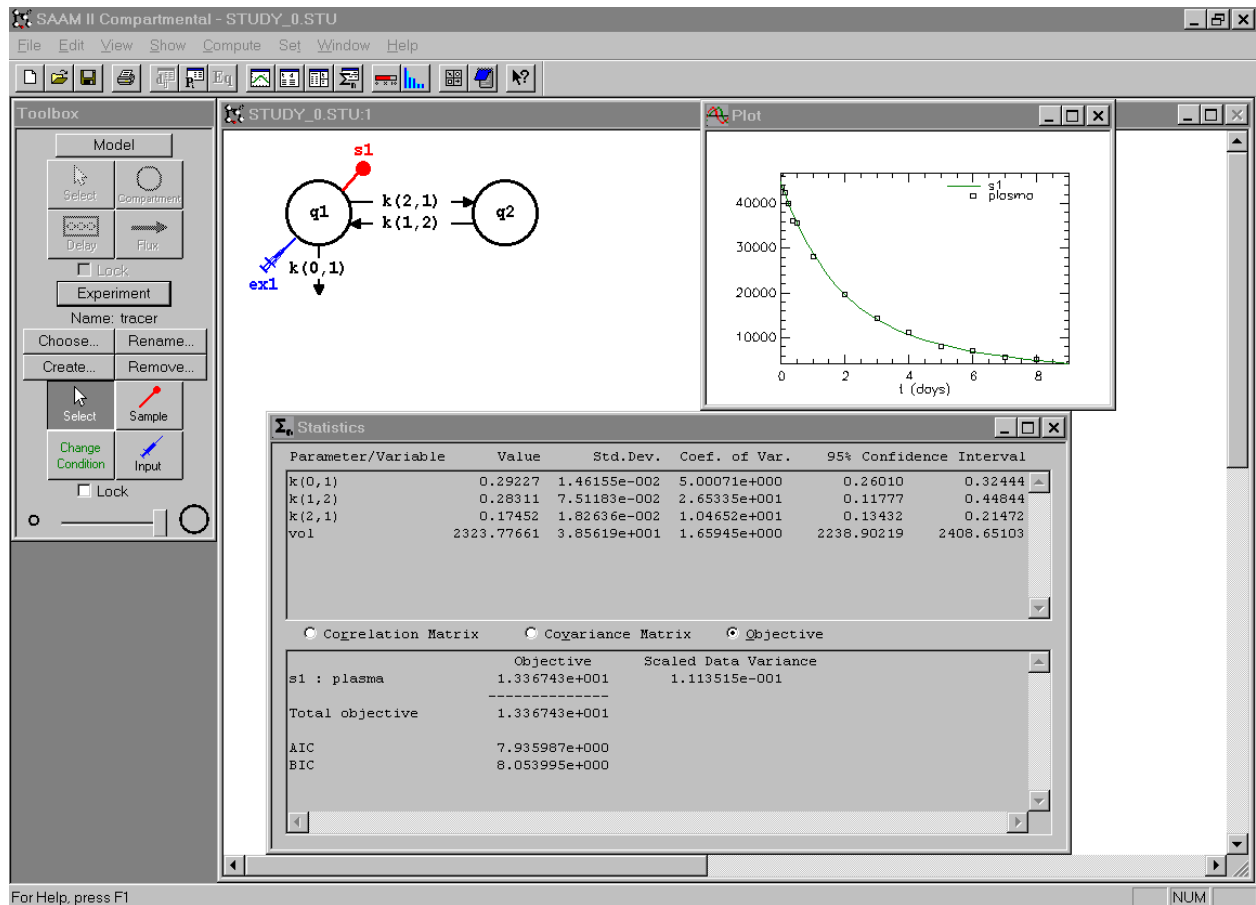
The SAAM II Toolbox:



The **SAAM II Toolbox** will be discussed in detail in the next part of this tutorial.

Take a minute to examine the various tools on the **SAAM II Toolbar** and in the **Toolbox**. Place the cursor on top of a **SAAM II** tool to show text describing the tool's function.

3. As you proceed through this tutorial, you will notice that several windows can be open at one time; this is normal and as you will see can be very helpful. An example is shown as follows:



In most cases in this tutorial, only the current window will be shown in the text. In the actual application, several windows may actually be open.

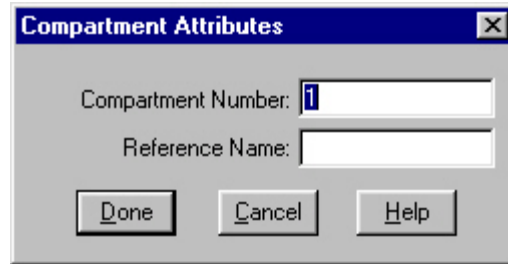
4. Dialog boxes associated with SAAM II objects.



Objects and dialog boxes. Every object on the **Drawing Canvas** has a dialog box associated with it.



- To open the dialog box associated with a particular object, simply double-click that object. For example, if you double-click **Compartment 1**, the **Compartment Attributes** dialog box for **Compartment 1** will open as shown below:



There is a box with the compartment number in it, and a box to add a reference name. If you wish, you can change the compartment number, or you can add a reference name such as “Plasma.” The reference name will appear in the circle that represents Compartment 1; it is for reference purposes only and is not used by the software.

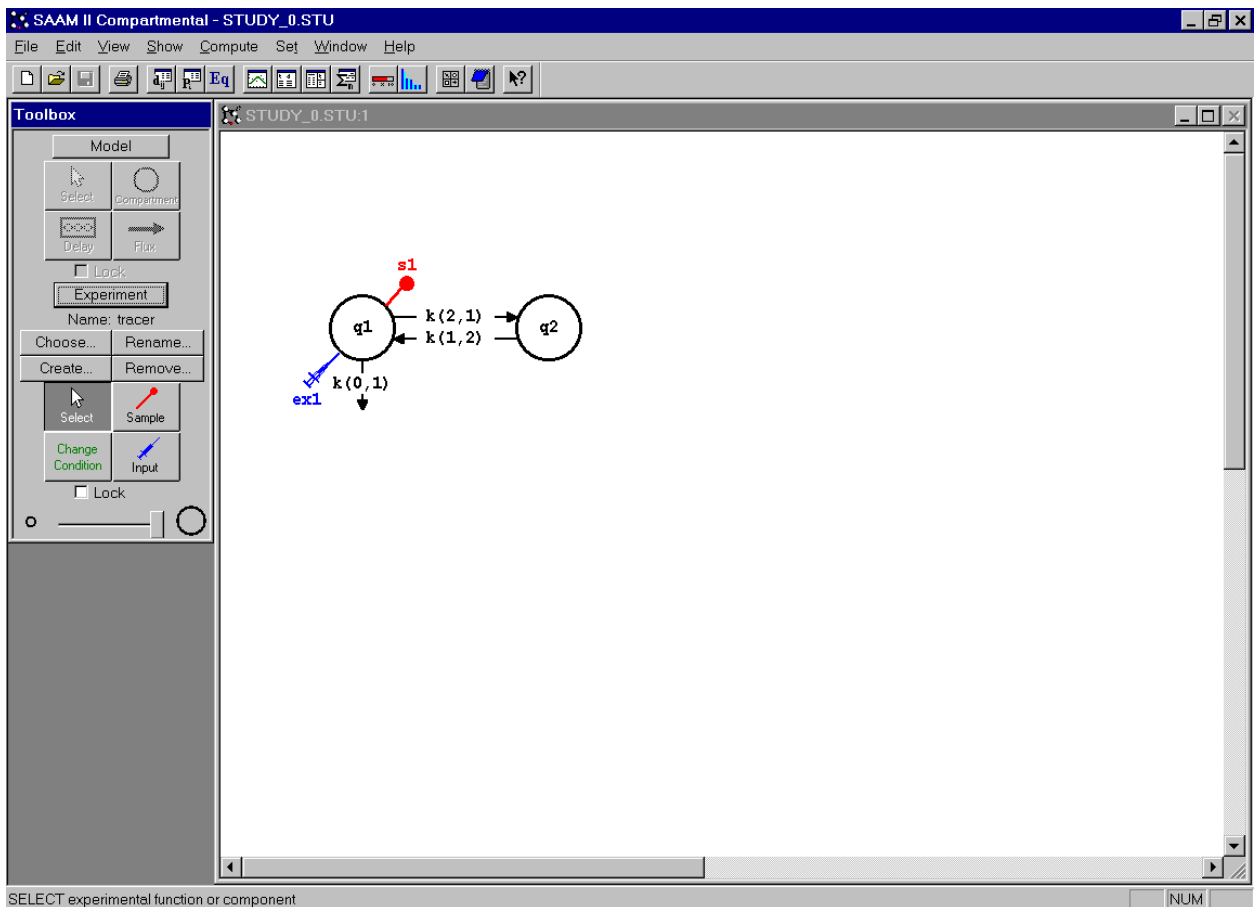
- b. To close the dialog box, click **Done**.
5. Open and investigate the experiment on the System Model.



Models of systems and models of experiments: It is very important to understand the **SAAM II** philosophy of separating the creation of the system model, i.e. how you believe your system functions in terms of a compartmental model, from duplicating an actual laboratory experiment on the model. As you will learn in Part 2, the **Model** tools in the **SAAM II Toolbox** allow you to build a model for the system, and the **Experiment** tools in the **SAAM II Toolbox** allow you to create an experiment on the system model.



- a. In the **SAAM II Toolbox**, click **Experiment**. The **SAAM II Compartmental** main window should appear as follows:



This is the model of the experiment. Notice that the compartment names have changed from **1** and **2**, to **q1** and **q2**. In SAAM II, **q1** and **q2** represent the differential equations created internally and solved by SAAM II. The input arrow **U(1)** is now replaced by the experimental input syringe, **ex1**, and there is a sample icon, **s1**, representing the experiment sample. The input arrow **U(1)** represents tracee input in a tracer-tracee experiment and will not be discussed in this tutorial.

- b. On the **Drawing Canvas**, double-click **ex1**. The **Exogenous Input** dialog box will appear as follows:

Exogenous Input

Name: Reference Name: Units:

Type	Initial	Constant	Start	Stop	Repeat Every	Nr. Repeats
Bolus	1.04e+8	-	0.000	-	-	-

Input Type:

Bolus
 Infusion
 Primed Infusion
 Equation

Initial Amount:

Constant Rate:

Event Start:

Event Stop:

Repeat Every:

Nr. of Repeats:

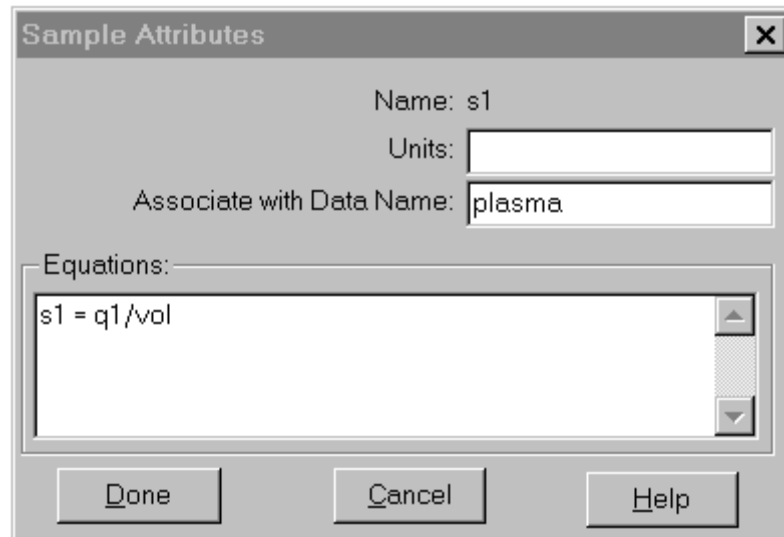
Equation:



Experiment inputs. There are many useful options for experiment inputs that you can specify in this dialog box. Several different types of input are possible: bolus, infusion, primed infusion, equation-described, repeated inputs, and split inputs. For this tutorial, a single bolus injection of $1.04e+08$ dpm (disintegrations per minute) is being used.



- c. To close the dialog box, click **Done**.
- d. On the **Drawing Canvas**, double-click **s1**. The **Sample Attributes** dialog box will open as follows:



Sample Attributes. There are many useful options for the experimental sample that you can specify in this dialog box.

The units of the experimental data, in this case dpm/ml, are for reference purposes only.

The **Associate with Data Name** box contains the name of the data in the data file associated with this sample. If you do not have a data name associated with a sample, and try to fit the model to the data, **SAAM II** will generate a warning message.

The sample equation in the **Equations** pane, in this case "s1=q1/vol", is the equation which links the solution of the differential equation **q1** with the data. Writing the sample equation is a fundamental step in building a model and adds a new parameter, *vol*, to the model.



- e. To close the dialog box, click **Done**.
6. View the data.

Data in **SAAM II** are entered in a text file where columns are space delimited. The data file for the study **study_0.stu** can be viewed as follows:

- a. In the **Show** menu, click **Data**, or alternatively, on the **SAAM II Toolbar** click **Data**



The **Data** window will open as follows:

```

DATA
(FSD 0.1)
t      plasma
0.007  46780
0.042  43522
0.125  42535
0.25   40125
0.375  36221
0.5    35562
1.0    28194
2.0    19573
3.0    14403
4.0    11278
5.0    8081
6.0    6999
7.0    5653
8.0    5139
9.0    4210
END

```

The first line of the data file is the word “DATA.” The next line, (FSD 0.1) specifies the weights assigned to the data. The first column in the data file is always the independent variable, usually time denoted *t*. The columns representing data can be named whatever you wish; the name is case sensitive. However, the name of this column must be the same as the name in the appropriate **Sample Attributes** dialog box.




Data weighting. Data weighting is used to provide a measurement of the user’s confidence in a particular datum and is used in the “fitting” process. Data weights are calculated as the inverse of the data variance. **SAAM II** contains several variance models. If no method is explicitly specified, a fractional standard deviation of 0.1 (FSD 0.1) is assigned as the variance model to each datum.

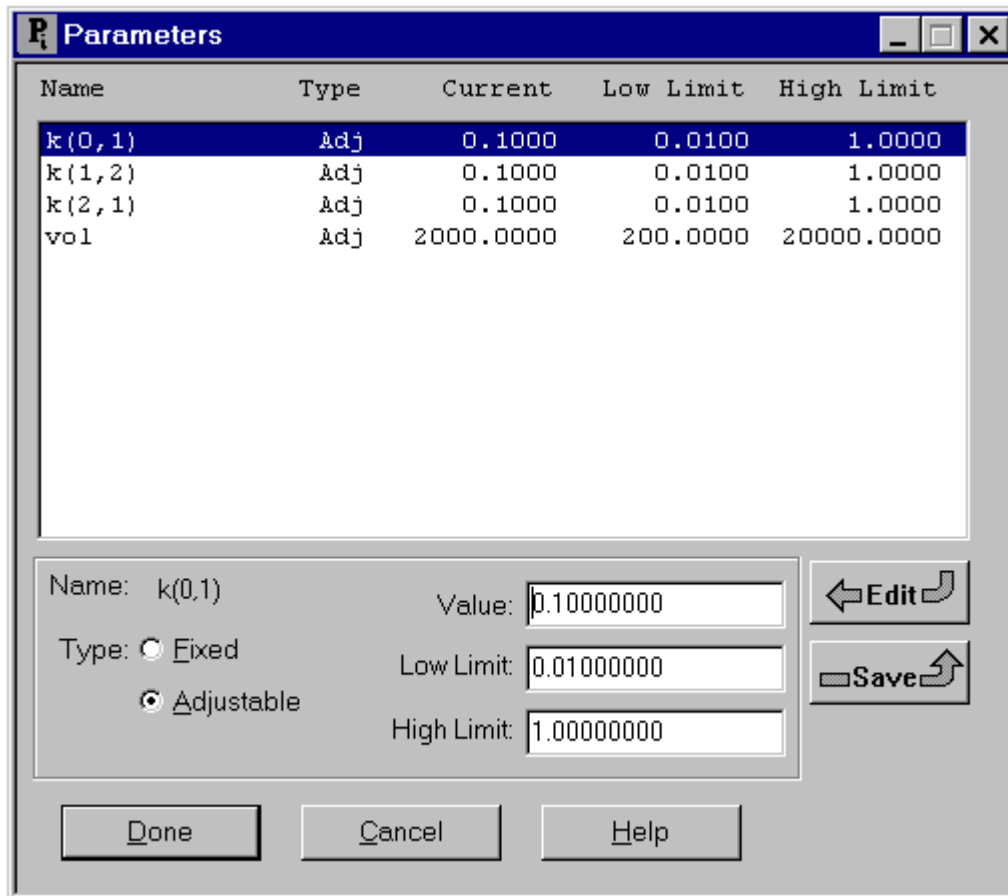
SAAM II calculates weight for each datum from the standard deviations you assign to your data. In the file above, the variance model, (FSD 0.1), means that a constant coefficient of variation (fractional standard deviation) of 10% is assigned to each datum. Therefore, for example, the standard deviation of the datum of 46780 is 4678.



- b. **Close** the Data window.
5. View the model parameters.

The model has four parameters: $k(2,1)$, $k(1,2)$, $k(0,1)$ and *vol*. These parameters are entered in the **Parameters** dialog box.

- a. In the **Show** menu, click **Parameters**, or alternatively, on the **SAAM II Toolbar** click **Parameters** . The **Parameters** dialog box will open as shown below:



Properties of parameters. There are several important features of the **Parameters** dialog box.


- i. Each parameter has a "Type" that is either "fixed" or "adjustable." A fixed parameter is a parameter that is assumed to be known and does not change when the model is "fitted" to the data. An adjustable parameter is adjusted when model is "fitted" to the data.
- ii. Each parameter, whether fixed or adjustable, has a "current" value; this is the value that will be used when you Solve or Fit the model.
- iii. Adjustable parameters have upper and lower limits. These are limits that cannot be exceeded when **SAAM II** Fits the model to the data. If **SAAM II** is Fitting the model to the data and a limit is reached, **SAAM II** will display a warning message.

- iv. To change a parameter value, double-click on the parameter name. Its current value, and high and low limits if it is adjustable, will be shown in the **Value**, **High Limit** and **Low Limit** boxes respectively. To save the changes, click **Save**.



- b. To close the **Parameters** dialog box, click **Done**.

6. Solve the model.

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



Solve. When you “Solve,” SAAM II uses the current values of the parameters to solve the system of differential equations represented by the compartmental model.

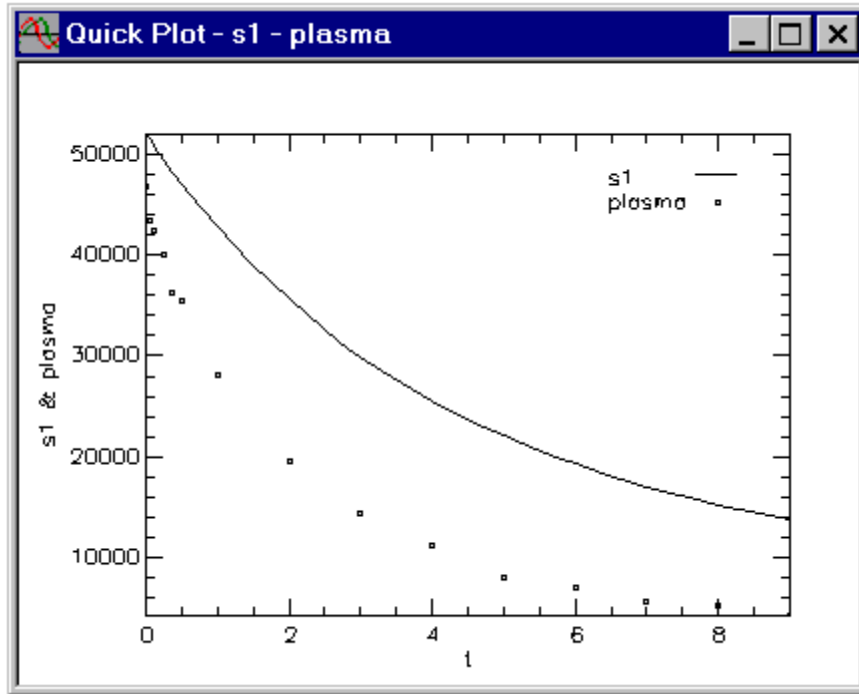
During a “Solve,” a **Solve Status** message will appear showing the status of the integration (solving). For small models such as this one, the message will appear and disappear extremely fast. For larger models, you can watch the progress. You can also choose to abort a “Solve.”



7. View the solution to the model using **Quick Plot**.

- a. On the **Drawing Canvas**, click **s1** to select it.
- b. In the **View** menu, click **Quick Plot**.

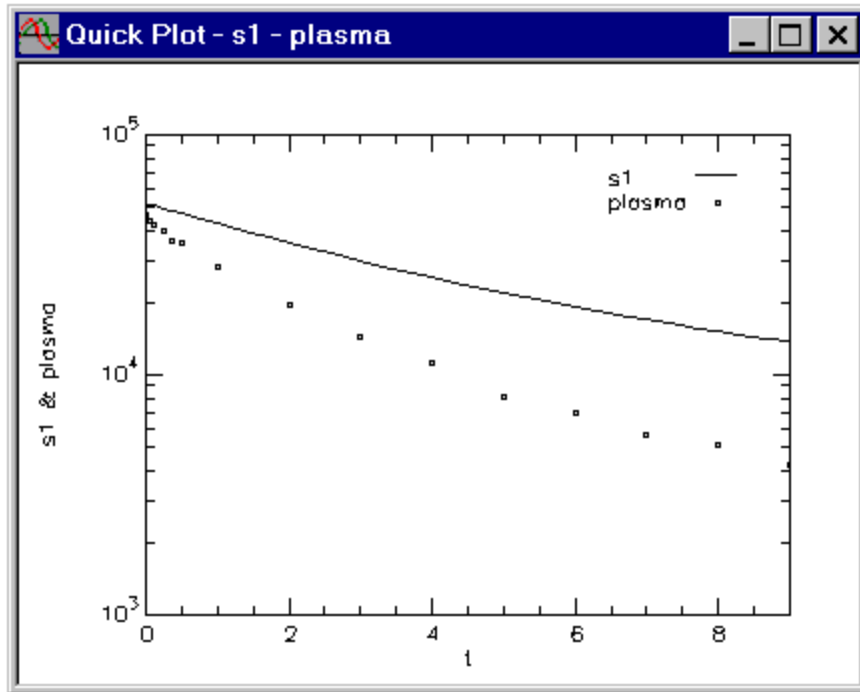
The following plot will appear in the **Quick Plot** window. Notice that the scale is linear.




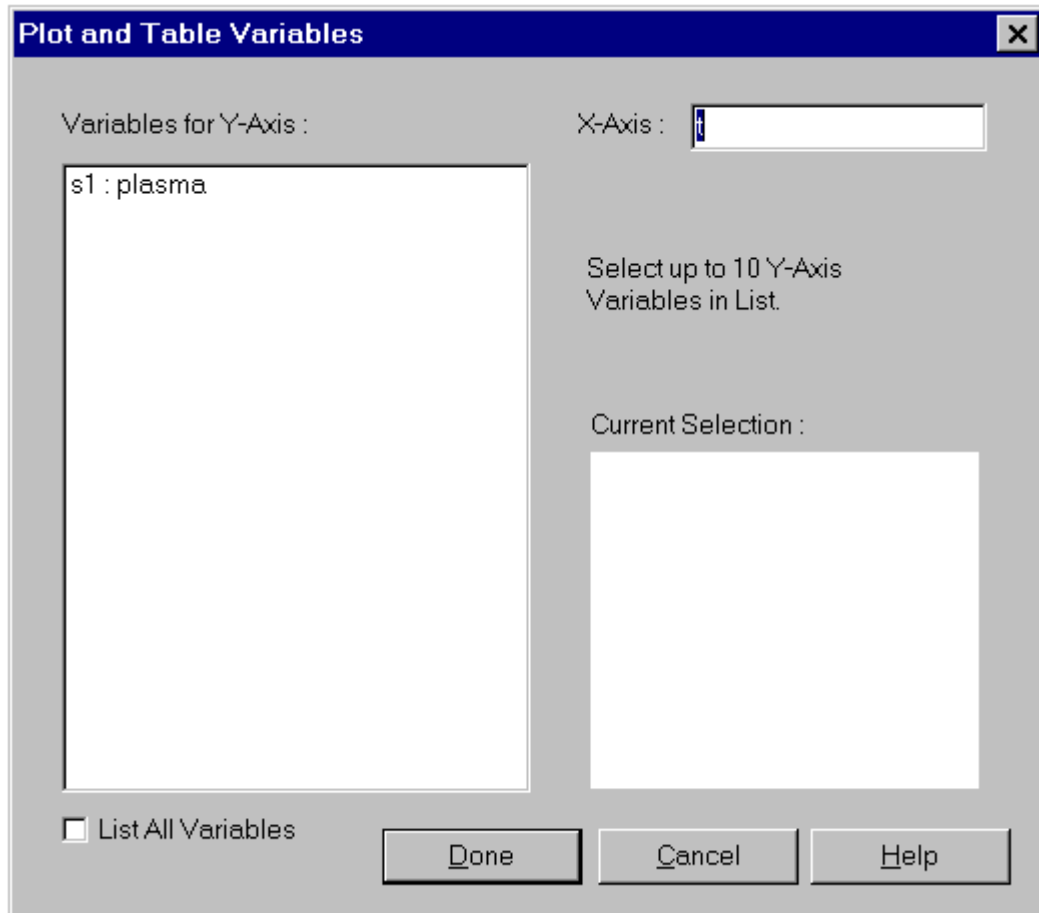
Quick Plot. **Quick Plot** has preset defaults that you cannot change. As you can see below, when you use the **Plot** command, you have more flexibility in what you can plot and how you can plot it.



- c. To view this plot in semi-logarithmic mode, in the **View** menu, click **Semilog**. The plot will appear as follows:

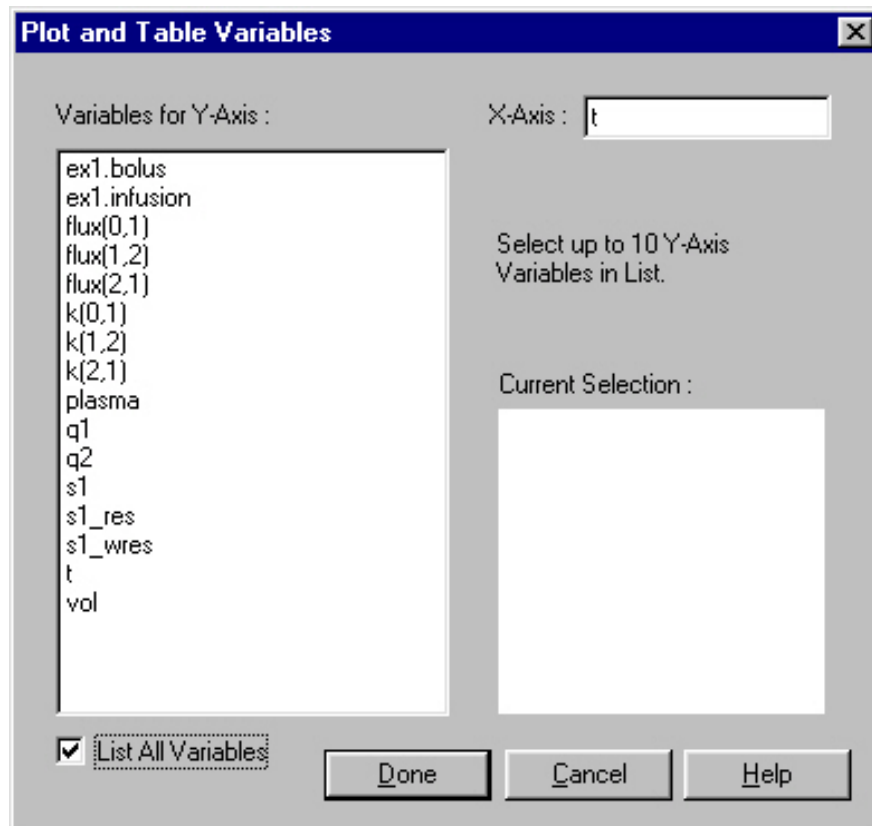


- d. Close the **Quick Plot** window.
8. View the solution to the model using the **Plot** command.
 - a. In the **Show** menu, click **Plot**, or alternatively, on the **SAAM II Toolbar** click **Plot** . The **Plot and Table Variables** dialog box will open as follows:



Only the variables that are associated with data will appear in the **Variables for Y-Axis** pane. However, you can plot any of the variables in the model as described below.

- b. In the **Plot and Table Variables** dialog box, select the **List All Variables** check box. All the variables that can be plotted will appear as follows:



You can now select among the different variables for the Y-Axis for the plot.

- c. In the **Plot and Tables** dialog box, clear the **List All Variables** check box to clear the Y-Axis variables except **s1:plasma**.
- d. In the **Variables for Y-axis** pane, click **s1:plasma**. The selection will move to the **Current Selection** pane.
- e. Click **Done**.

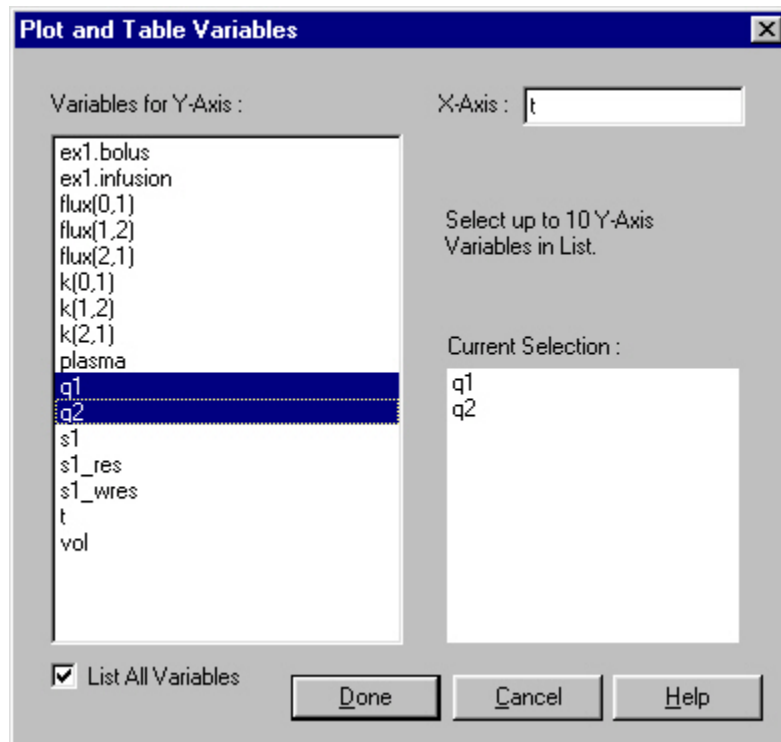
A plot similar to the previous **Quick Plot** will appear.

9. Change the plot variables.

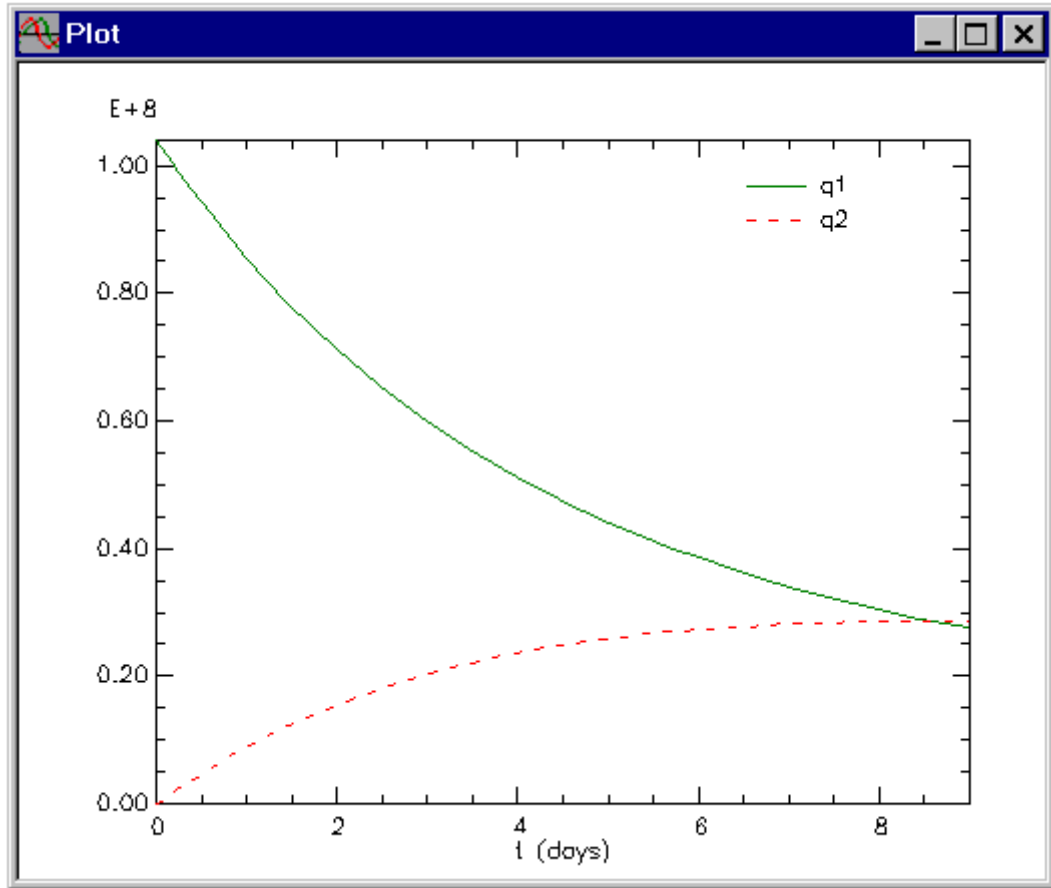
SAAM II will remember the plot variables, e.g. **s1:plasma** when you open and shut the **Plot** window. If you want to change the plot variables, you need to change the variable names using the **Plot and Table Variables** dialog box in the **Set** menu while a **Plot** window is open. The following will illustrate how to plot **q1** and **q2** so you can compare the model solution for these two variables.

- a. With the **Plot** window open, in the **Set** menu, click **Plot/Table Variables**. The **Plot and Table Variables** dialog box will open.

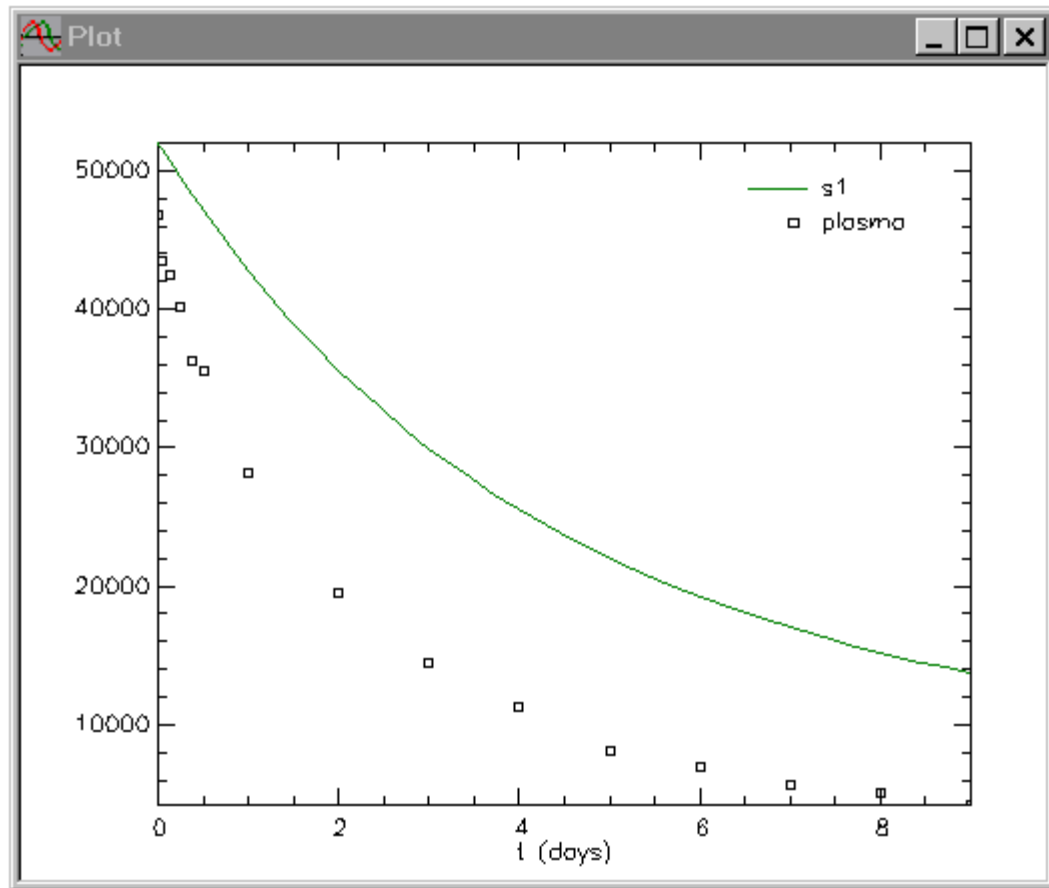
- b. Select the **List All Variables** check box (notice **s1** and **plasma** are selected).
- c. In the **Variable for Y-Axis** pane, click **q1**; q1 moves to the **Current Selection** pane.
- d. Press the **CTRL** key and click **q2**; q2 moves to the **Current Selection** pane. (Pressing the **CTRL** key allows you to select multiple items). The **Plot and Table Variables** dialog box will appear as shown below:



- e. Click **Done**. The plot will appear as follows:



- f. With the **Plot** window open, in the **Set** menu click **Plot/Table Variables**. The **Plot and Table Variables** dialog box will open. Clear the **List All Variables** check box. In the **Variables for Y axis** pane, click **s1:plasma**, then click **Done**. The **Plot** window will appear as follows:



10. Fit the model to the data.

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



Leaving the Plot window open. The **Plot** window can remain open during a “Solve” or “Fit.” The plot will be updated after a successful “Solve” or “Fit.”

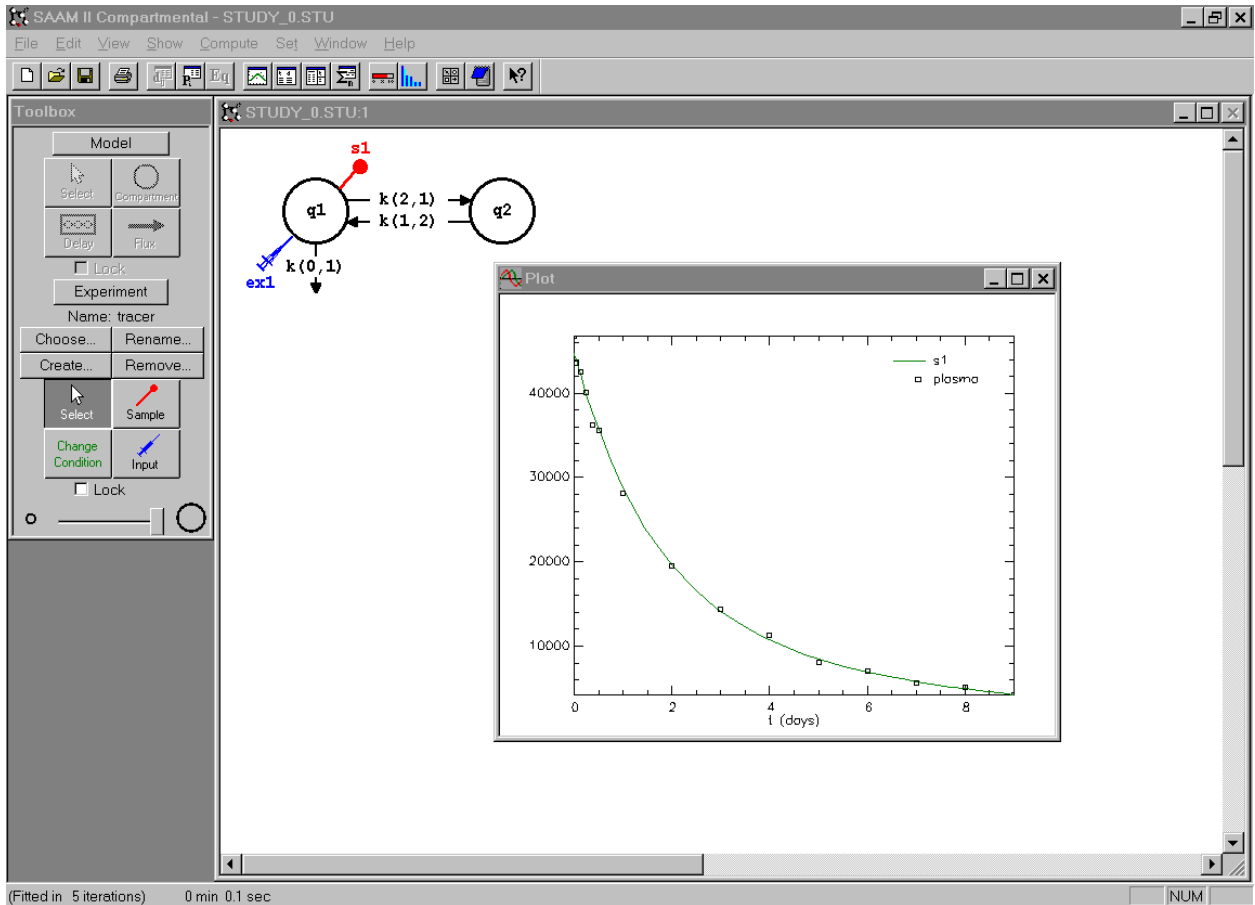


Fit status. During a “Fit,” a **Fit Status** message will appear (on a fast computer, you may just see a flash). This is the counterpart to the **Solution Status** message you saw when you solved the model originally. The **Fitting Status** bar gives information both

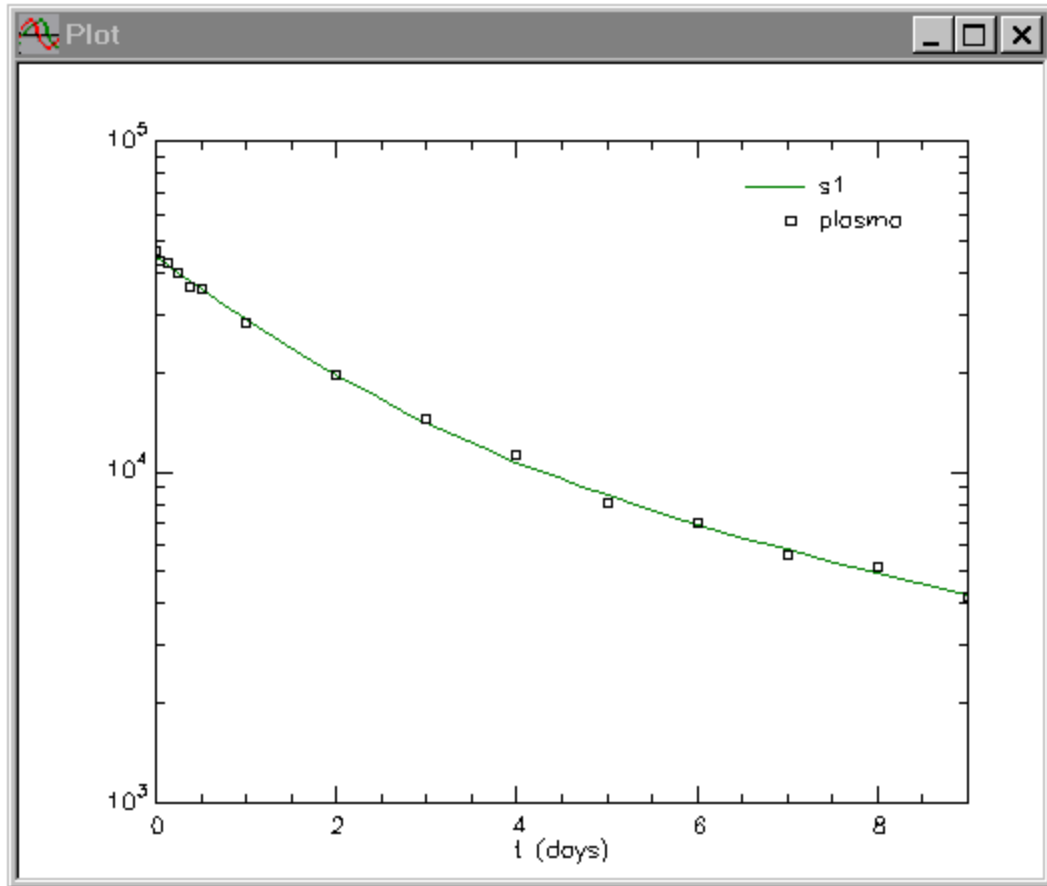
on the integration part of the “Fitting” and on the number of iterations. You can abort the “Fit” by clicking **Abort**.




When you have Fitted the model to the data, the **SAAM II Compartmental** main window should appear with the **Plot** window as follows:



The new parameter values will replace the original estimates in the **Parameters** dialog box, and the best fit of the model to the data appears in the plot. (You can change the plot to semi-logarithmic if you wish by clicking **Semilog** in the **View** menu - this is possible because the **Plot** window is open.) The semilog plot will appear as follows:



11. View the statistics associated with the “Fit.”

- a. In the **Show** menu, click **Statistics**, or alternatively on the **SAAM II Toolbar** click **Statistics** . The **Statistics** window will appear as follows:

Parameter/Variable	Value	Std.Dev.	Coef. of Var.	95% Confidence Interval	
k(0,1)	0.29227	1.46155e-002	5.00071e+000	0.26010	0.32444
k(1,2)	0.28311	7.51183e-002	2.65335e+001	0.11777	0.44844
k(2,1)	0.17452	1.82636e-002	1.04652e+001	0.13432	0.21472
vol	2323.77661	3.85619e+001	1.65945e+000	2238.90219	2408.65103

Correlation Matrix
 Covariance Matrix
 Objective

	Objective	Scaled Data Variance
s1 : plasma	1.336743e+001	1.113515e-001
Total objective	1.336743e+001	
AIC	7.935987e+000	
BIC	8.053995e+000	



Statistical information following a successful “Fit.” The **Statistics** window contains information about the “Fit.” It includes

- i. the final values for the parameters, their estimated standard deviation, percent coefficient of variation, and 95% confidence interval.
- ii. the following objective function information:
 - Final value of the objective function (this is the function that is minimized during the fitting process)
 - Scaled data variance (this is a number that is estimated during the fitting process when you use relative weighting – the default option in SAAM II)
 - Values for AIC and BIC; these values are used in the model development process to help assess which model structure best fits the data.
- iii. the Covariance matrix.
- iv. the Correlation matrix.

If, for example, in the **Statistics** window, you select the **Correlation Matrix** option, the Correlation Matrix will appear in the lower half of the **Statistics** window. The Covariance Matrix or the values for the Objective will appear if you select one of these other options.



- b. Close the **Statistics** window.
- c. Close the **Plot** window.

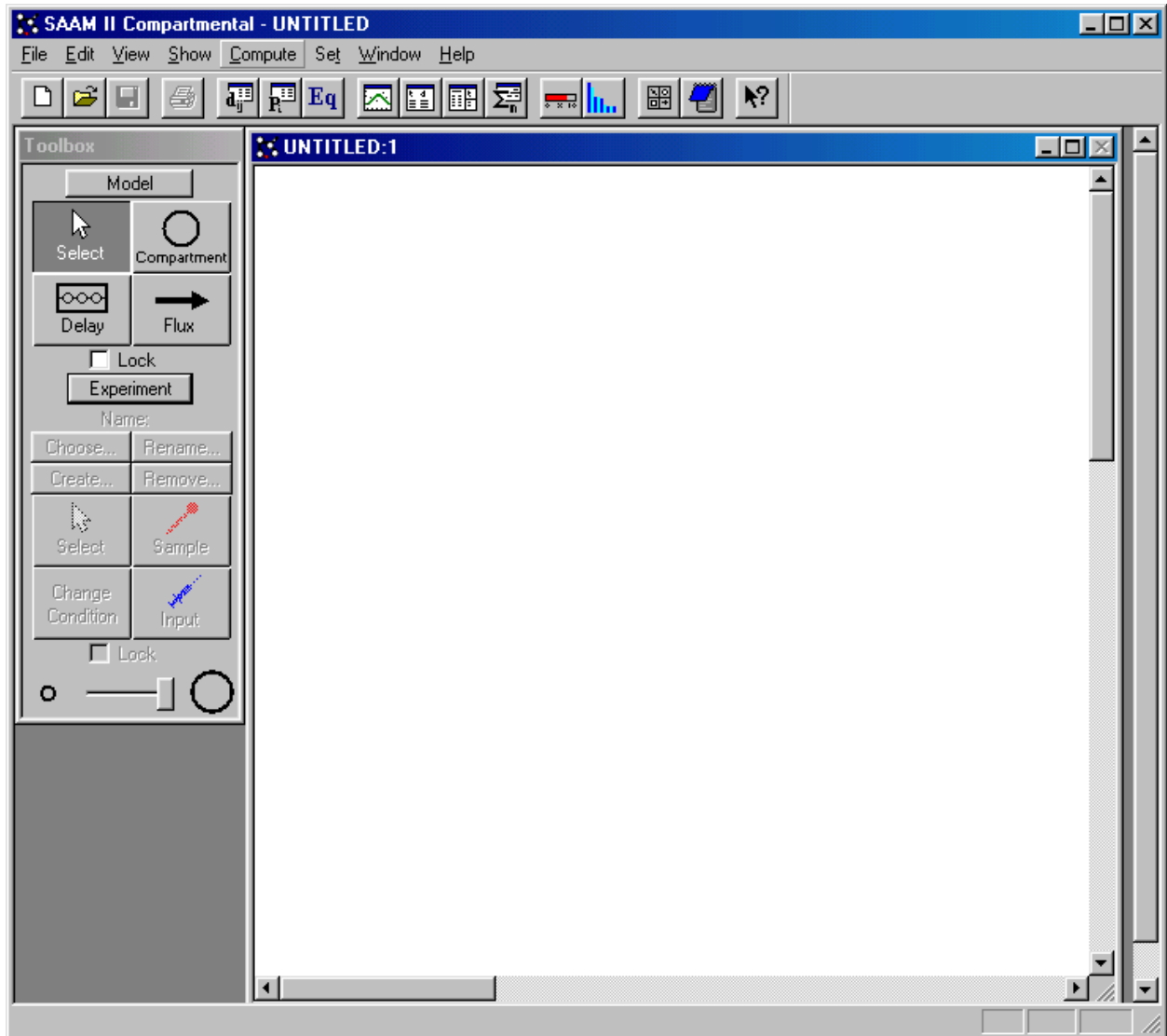
12. **Quit the SAAM II Compartmental** application

- a. In the **File** menu, click **Exit**.
- b. Click **No** (you do not wish to save the file).

Part 2. Building models and creating experiments in the SAAM II Compartmental application.

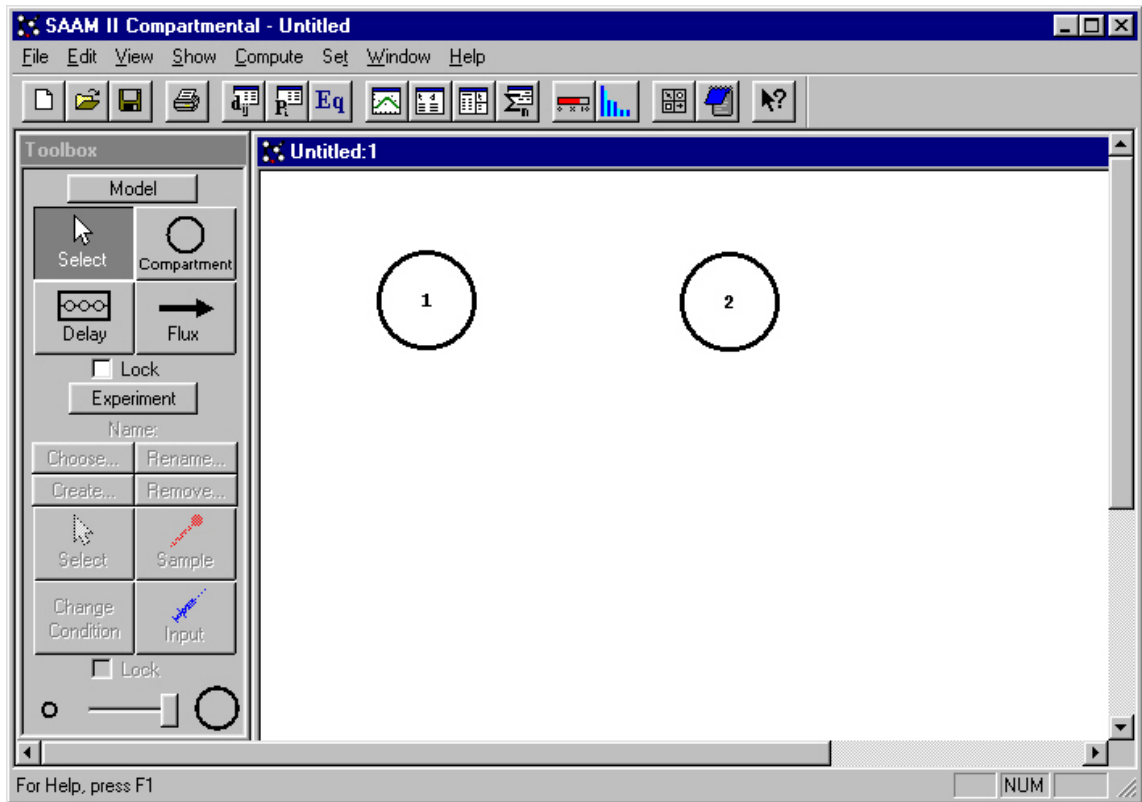
This part of the tutorial will show you how to build the two-compartment model and conduct the experiment on the model used in Part 1. This part of the tutorial will show you how to use the **Model** and **Experiment** tools in the **SAAM II Toolbox** for building system models and creating experiments on the models.

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



2. Create the two compartments of the two-compartment model.
 - a. In the **SAAM II Toolbox**, click **Model**. (This ensures that the **SAAM II Model** building tools are available.)
 - b. In the **SAAM II Toolbox**, click **Compartment** (this tool is now available).
 - c. Click on the **Drawing Canvas** approximately where you would like the first compartment to be located. A compartment with the number **1** will appear on the **Drawing Canvas**.
 - d. Click **Compartment** in the **SAAM II Toolbox** a second time (this tool is again available).
 - e. Click on the **Drawing Canvas** approximately where you would like the second compartment to be located. A compartment with the number **2** will appear on the

Drawing Canvas. The SAAM II **Compartmental** main window should appear as shown below:



Locking Tools. If you know you are going to be creating several compartments for the model, you can lock the **Compartment** tool so it is available until you unlock it. For example, to facilitate building a multi-compartmental model, you can do either of the following:

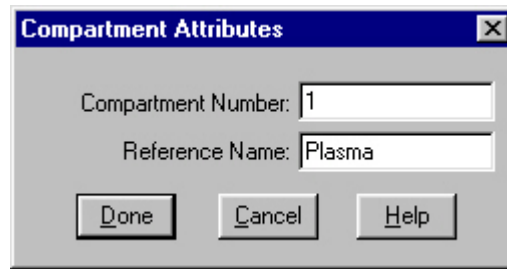
- i. In the **SAAM II Toolbox**, double-click **Compartment** to lock the tool, or
- ii. In the **SAAM II Toolbox**, click **Compartment**, and then select the **Lock** check box at the bottom of the **SAAM II Toolbox**.

The **Compartment** tool will be available until you unlock it by clicking **Select** in the **SAAM II Toolbox**.



Objects and Dialog Boxes. Remember, every object on the **SAAM II Compartmental Drawing Canvas** has a dialog box associated with it. Double-click

compartment **1** to open the **Compartment Attributes** dialog box associated with this compartment. Type “Plasma” in the **Reference Name** box as shown below:



Click close the dialog box, click **Done**. Note the word “Plasma” appears in the circle that represents Compartment **1**.



3. Construct transfers between Compartments **1** and **2**.
 - a. In the **SAAM II Toolbox**, double-click **Flux** (notice that double-clicking will lock the **Flux** tool so you can perform multiple operations).
 - b. On the **Drawing Canvas**, click on Compartment **1**, and then click on Compartment **2**.

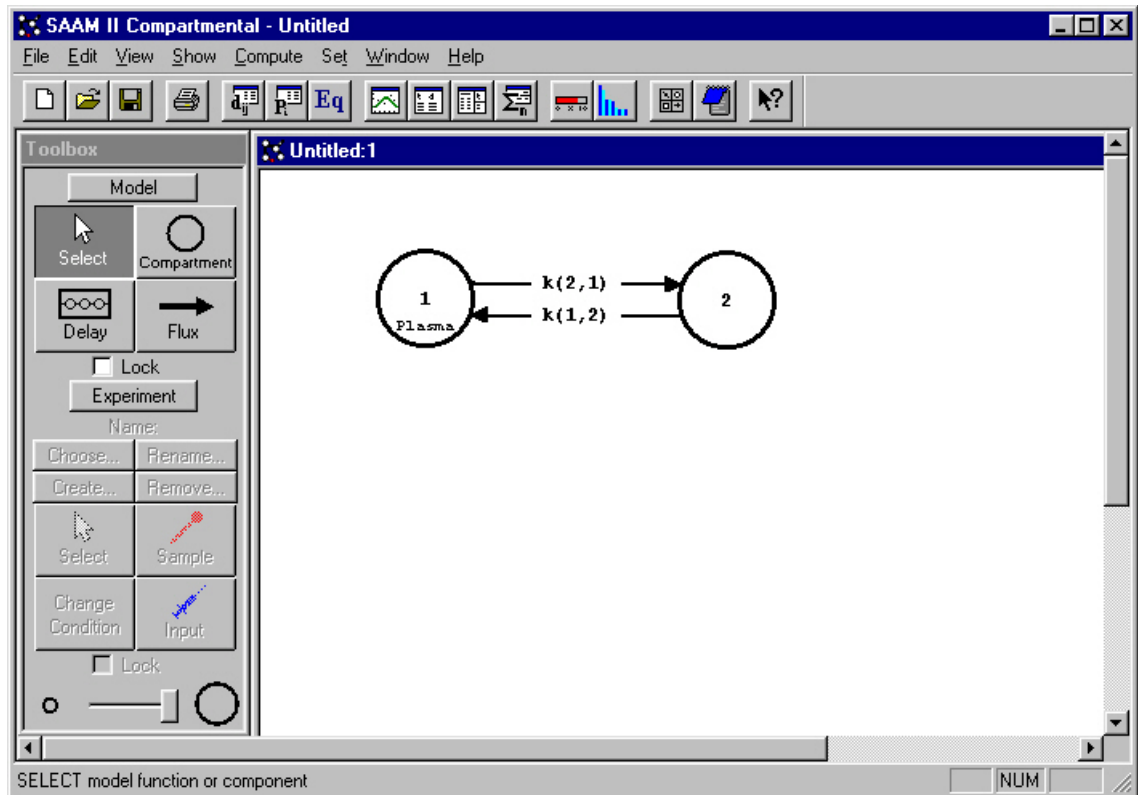
A flux (transfer) arrow to Compartment **2** from Compartment **1** that is labeled $k(2,1)$ is created. If the label does not appear, it is because Compartments **1** and **2** are too close to each other. If this is the case, move Compartment **2** farther away from Compartment **1**.

- c. On the **Drawing Canvas**, click on Compartment **2**, and then click on Compartment **1**.

A flux (transfer) arrow to Compartment **1** from Compartment **2** that is labeled $k(1,2)$ is created.

- d. In the **SAAM II Toolbox**, click **Select**. The **Flux** tool is no longer available.

The SAAM II **Compartmental** main window should appear as shown below:



Notice, as described above, Compartment 1 has been given the reference name “Plasma.”



Creating transfers. To create a transfer between, for example, Compartment 1 and 2, with the **Flux** tool available, you can click on Compartment 1 and drag to Compartment 2.



4. Construct losses from Compartments 1 and 2.
 - a. In the **SAAM II Toolbox**, double-click **Flux**.
 - b. On the **Drawing Canvas**, click on Compartment 1, and then click anywhere on the canvas.

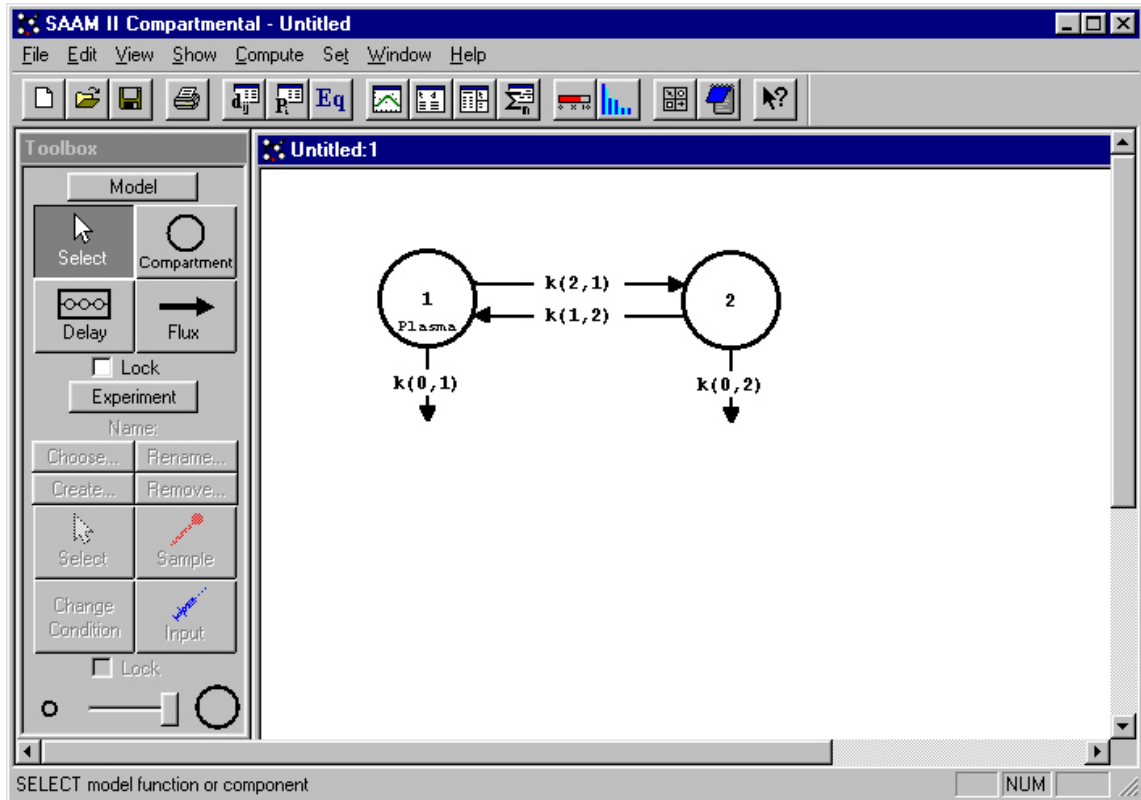
This will create a loss, $k(0, 1)$, from Compartment 1. No matter where you click on the **Drawing Canvas**, the loss will always point down.

- c. On the **Drawing Canvas**, click on **Compartment 2**, and then click anywhere on the canvas.

This will create a loss, $k(0,2)$, from **Compartment 2**.

- d. In the **SAAM II Toolbox**, click **Select**. The **Flux** tool is no longer available.

The SAAM II **Compartmental** main window should appear as follows:

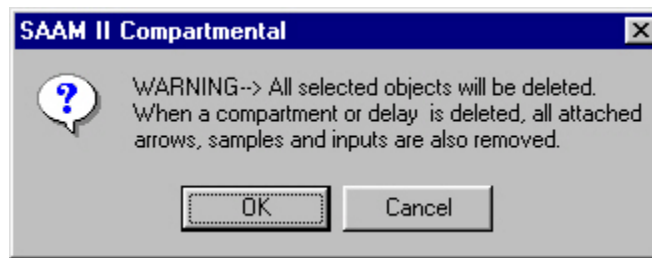


*Moving or nudging a compartment on the **Drawing Canvas**.* Suppose after you have created the model you want to move or nudge a compartment on the **Drawing Canvas** to line it up with another object. To move an object, click the compartment or delay you wish to move, and drag the object to where you would like it to be located on the **Drawing Canvas**. To nudge an object (e.g. to straighten transfer arrows), click the compartment you wish to nudge, and nudge it using the directional arrows on the keyboard.



Correcting a mistake by deleting an object. Suppose you accidentally add an object to the model by mistake. To delete the object from the **Drawing Canvas**:

- i. On the **Drawing Canvas**, click the object you wish to delete.
- ii. Either press the **Delete** key, or in the **Edit** menu, click **Delete**. The following warning message will appear as follows:



- iii. Click **OK** if it is okay, otherwise click **Cancel**.



Deleted Objects. When a compartment or delay is deleted, all attached arrows, experimental samples and inputs are also deleted!



5. Delete the loss $k(0,2)$ from the model.
 - a. On the **Drawing Canvas**, click $k(0,2)$ to select it.
 - b. Press the **Delete** key.
 - c. Click **OK**.

This will delete the loss $k(0,2)$ from the model.

At this point, you have successfully created the two-compartment system model with a single loss from Compartment 1 used in Part 1. You now want to reproduce the experiment performed in the laboratory on this model. This point emphasizes the difference between building the system model and creating an experiment on the model. Obviously, as you can see below, there are many different experiments that can be created on the model. The main differences are where and how inputs are made, and where and how samples are taken. Separating the system from the experiment permits maximum flexibility in using the tools in the **SAAM II Toolbox**.

6. Create the experiment.
 - a. In the **SAAM II Toolbox**, click **Experiment**. Notice that the **Model** tools are unavailable and the **Experiment** tools are available.

The **Experiment Attributes** dialog box will open as follows:

Experiment Attributes

Independent Variable:

Units:

Start at:

End at:

- b. Change the entry in the **Units** box from “minutes” to “days.”
- c. Enter “9” in the **End at** box. The **Experiment Attributes** dialog box will appear as shown below:

Experiment Attributes

Independent Variable:

Units:

Start at:

End at:

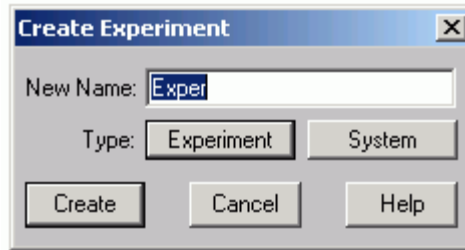


Experiment Attributes. The **Experiment Attributes** dialog box is normally where you set the ending time of the experiment. **Units** are for convenience only. **Start at** is normally zero which is the time of the first test input. **End at** is normally the time at which the experiment ends. There are, however, occasions when you may wish to set **End at** to a larger value.



- d. Click **Done**.

The **Create Experiment** dialog box will appear on the **Drawing Canvas**. The choice of experiment **Types** is an **Experiment** or a **System**. **Experiment** is selected. The **New Name** is “Exper” as shown in the following:



- e. Click **Create**.



Experiment vs. System. The **Create Experiment** dialog box is where you create your experiment. There are two types of experiments - “Experiment” and “System”.

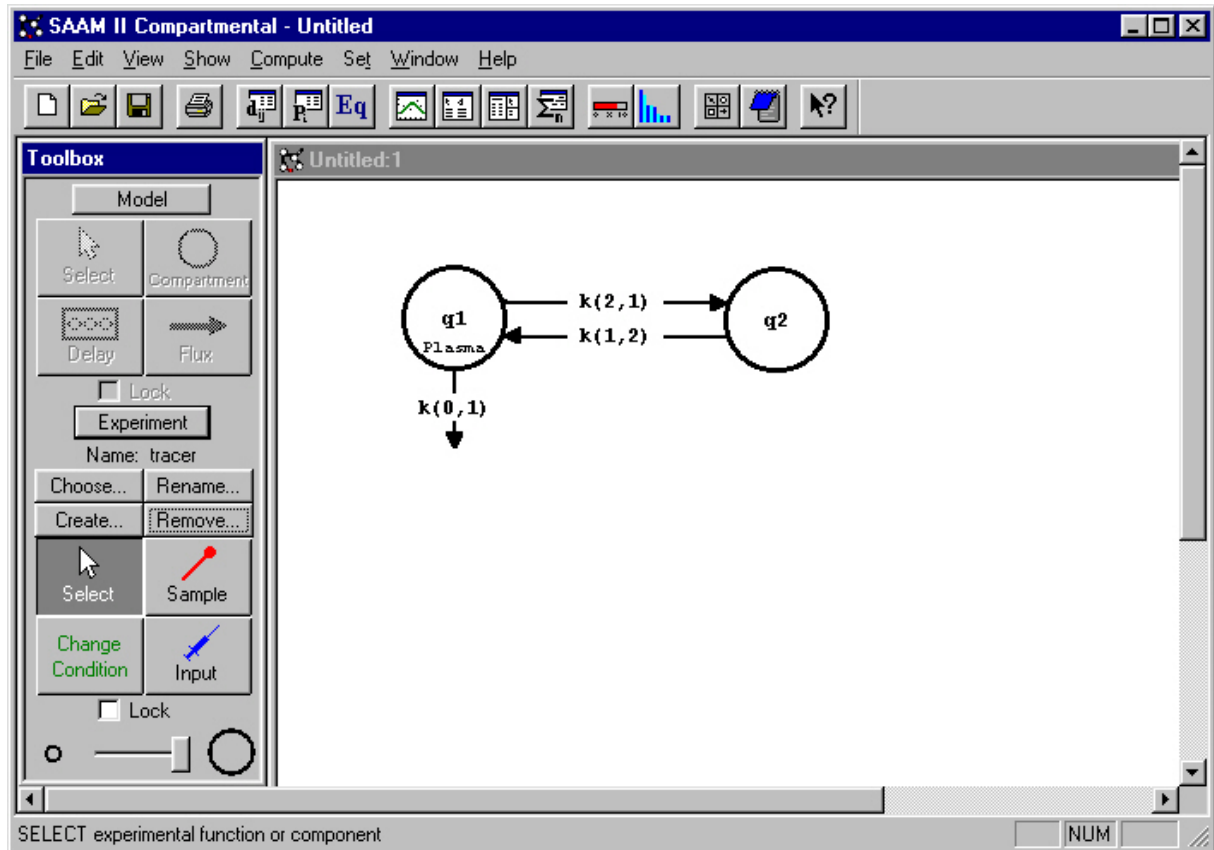
The **Experiment** type will invoke SAAM II’s differential equation machinery. When you create this type of experiment, your compartmental model will be interpreted by SAAM II as a system of differential equations. Once parameter values and inputs have been specified, SAAM II can Solve the system of differential equations, and can Fit your model to your data. This type of experiment is designed to deal with time dependent data following an experimental (exogenous) input into the system.

The **System** experiment creates a system of algebraic equations whose coefficients are the $k(i,j)$ of your compartmental model. The System model is used primarily in tracer-tracee experiments to describe the tracee data in the steady-state.

The default **New Name** is “Exper”. This can be changed to a name of your choice.



- f. The **SAAM II Compartmental** main window should appear as follows:



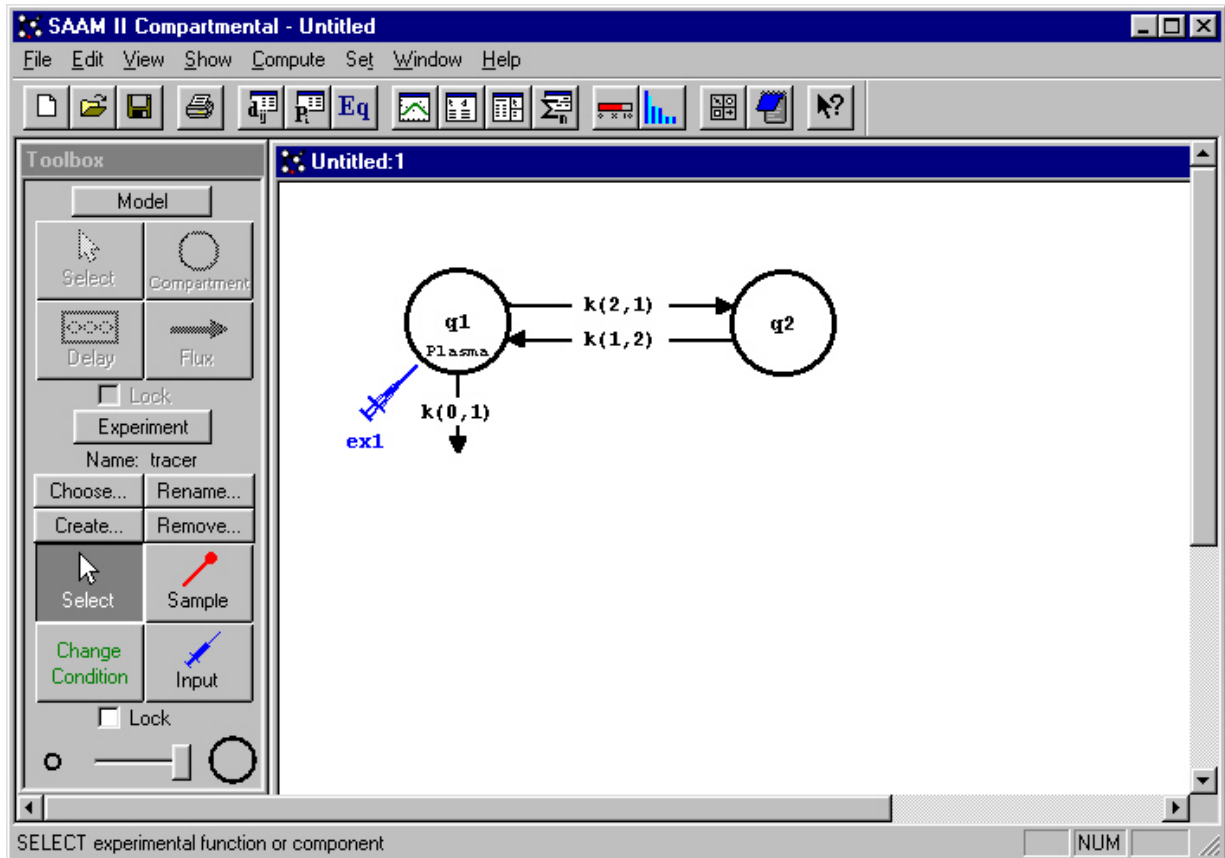
SAAM II Notation. Remember the model looks like the original model except now the compartment numbers have changed from 1 and 2 to **q1** and **q2**. Here **q1** and **q2** represent the solutions to the differential equations **q1'** and **q2'** created internally by **SAAM II**. The **q1** and **q2** are the calculated masses of experimental inputs into the two compartments at time t .



To recreate your laboratory experiment on the model, you need to specify the site and amount of your experimental input, the site of your measurement, and specify the measurement equation.

7. Add an experimental input to the model.
 - a. In the **SAAM II Toolbox**, click **Input**.
 - b. On the **Drawing Canvas**, click Compartment **q1**, and then click on the canvas.

An input arrow named **ex1** will appear on the **Drawing Canvas** pointing to Compartment **q1**. The **SAAM II Compartmental** main window should appear as follows:



- c. Double-click **ex1**. The **Exogenous Input** dialog box will open.
- b. Enter "1.04e+08" in the **Initial Amount** box.
- e. Click **Add**. The **Exogenous Input** dialog box should appear as follows (this is identical to the **Exogenous Input** dialog box you viewed in Part 1):

Exogenous Input

Name: Reference Name: Units:

Type	Initial	Constant	Start	Stop	Repeat Every	Nr. Repeats
Bolus	1.04e+8	-	0.000	-	-	-

Input Type:

Bolus
 Infusion
 Primed Infusion
 Equation

Initial Amount:
Constant Rate:
Event Start:
Event Stop:
Repeat Every:
Nr. of Repeats:

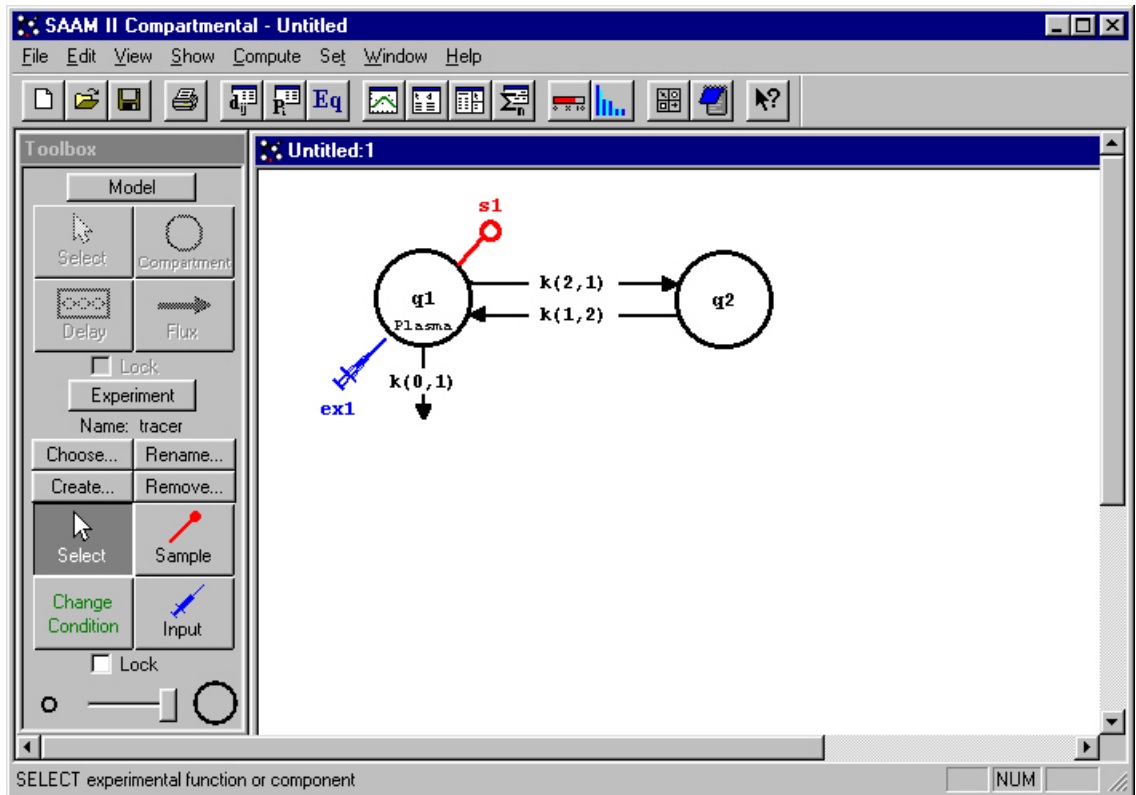
Equation:

Buttons: Save, Edit, Add, Delete, Split Input..., Done, Cancel, Help

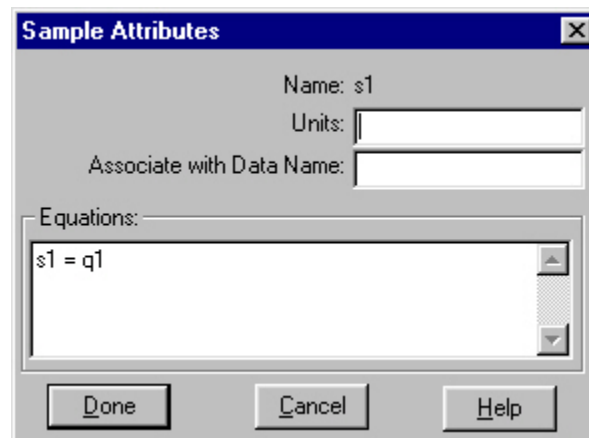
- f. Click **Done**.
9. Create a sample on the model. This sample will represent the sample you collected in your actual experiment.
- In the **SAAM II Toolbox**, click **Sample**.
 - On the **Drawing Canvas**, click Compartment **q1**, and then click on the canvas.

A sample object, **s1**, will appear on the **Drawing Canvas** attached to Compartment **q1**. This means your sample was from plasma. Notice that the circle at the top of the sample object is an open circle. The sample object can be moved on the **Drawing Canvas** as described above.

The SAAM II **Compartmental** main window should appear as shown below:



- c. On the **Drawing Canvas**, double-click **s1** to open the **Sample Attributes** dialog box as shown below:



- d. Type “plasma” in the **Associate with Data Name** box. As discussed in more detail below, “plasma” is the name of the data in the data file.
- e. Edit the sample equation “ $s1 = q1$ ” to read “ $s1 = q1/vol$ ” in the **Equations** pane. As discussed below, *vol* will become a new parameter in the model.

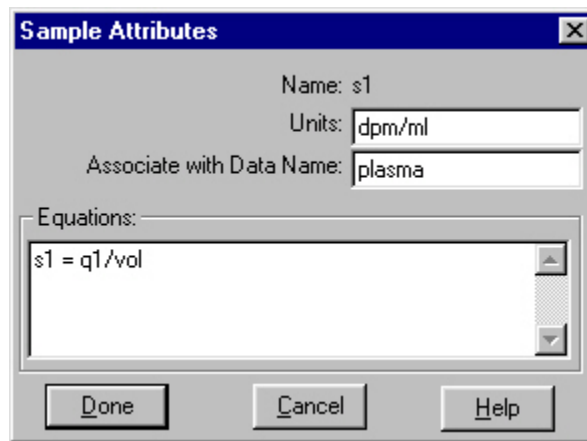


The Sample Equation. The sample equation, in this case “ $s1 = q1/vol$ ”, is what links the solution to the differential equations, the $q1$ and $q2$, with the data. The units of the differential equations are determined by the units of the input, $ex1$. The units of your data are usually concentration. Thus the sample equation keeps the units of the differential equations and the units of the data consistent.

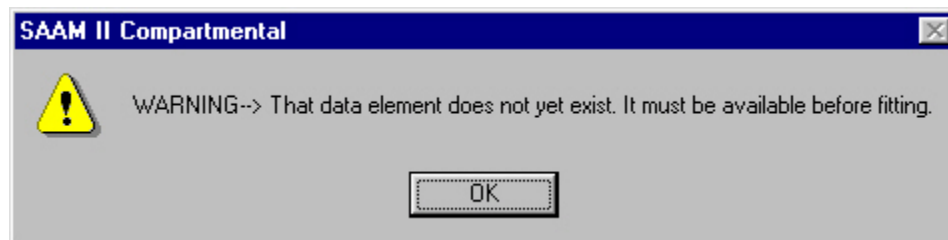


- f. If you wish, you can type “dpm/ml” in the **Units** box; this will be for bookkeeping purposes only.

The **Sample Attributes** dialog box will appear as shown below:



- g. Click **Done**. A warning message will appear because you have not entered your data yet. This warning message is shown below:



- h. Click **OK**.



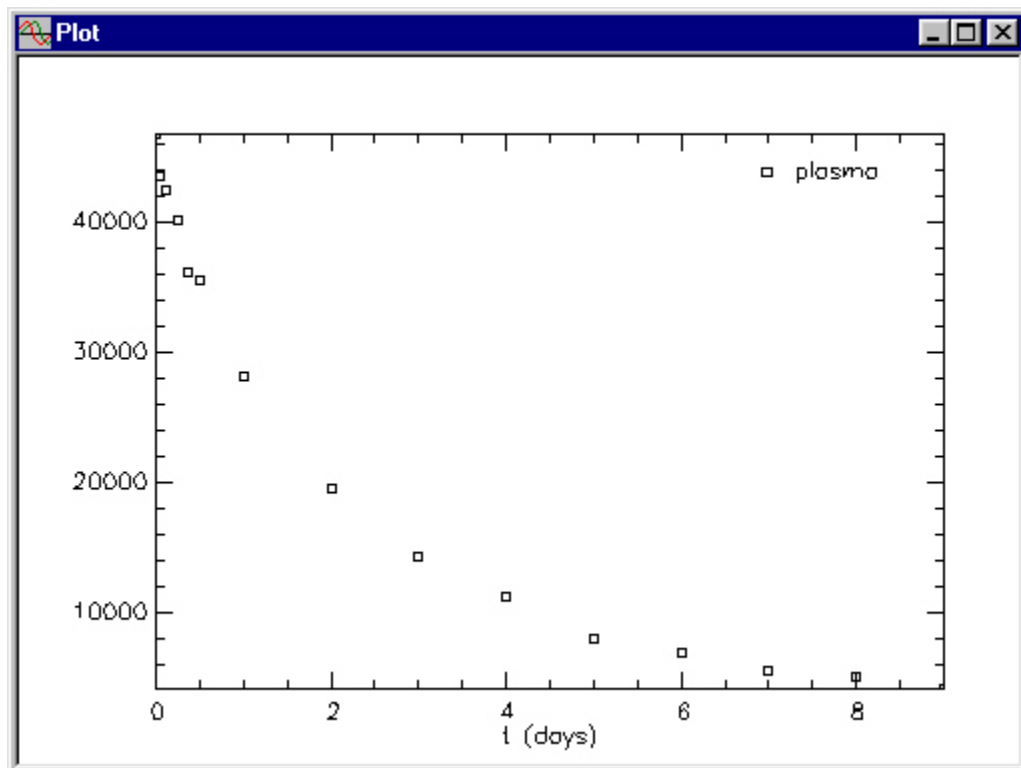
Sample Attributes. There are a number of important points to be made here that will help you when you use the **SAAM II Compartmental** application:


- i. When you close the **Sample Attributes** dialog box, you will get a warning message that the data element, i.e. the data named “plasma,” does not exist yet. This is because you have not yet entered your data. If you had entered the data first, and your data contained a column named “plasma,” you would not get this message.
- ii. The data name in **SAAM II** is case sensitive. Thus “Plasma” and “plasma” will be read as two different names.
- iii. The circle at the top of the Sample object will be solid when there is a data name associated with the sample. This is used as a modeling aid to help remind you when data associations were made.
- iv. The sample equation “ $s1 = q1/vol$ ” introduced a new parameter *vol* for the volume of Compartment **q1**.

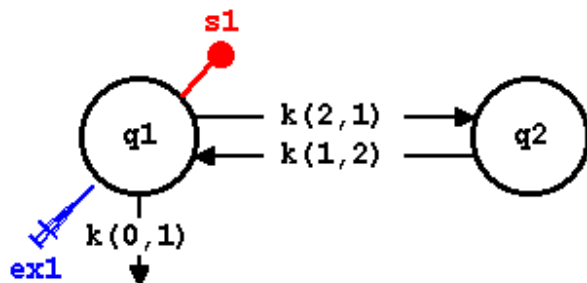


10. Add the data to the **SAAM II Compartmental** model.

The data you will use in **study_0** are shown below. These are decaying data following the bolus injection of a radio-labeled protein. A plot of these data is shown below:



- On the **Show** menu, click **Data**, or alternatively, on the **SAAM II Toolbar**, click **Data** . The **Data** window will open.
- On the **File** menu, click **Open**. The file **study_0.dat** should appear in the list (if it does not, find the folder where you put this data file).
- Double-click **study_0**. The data in this file will appear in the **Data** window. The model and the **Data** window should appear on the **Drawing Canvas** as follows:



t	plasma
0.007	46780
0.042	43522
0.125	42535
0.25	40125
0.375	36221
0.5	35562
1.0	28194
2.0	19573
3.0	14403
4.0	11278
5.0	8081
6.0	6999
7.0	5653
8.0	5139
9.0	4210

END

Data Format is okay

- Close the **Data** window.




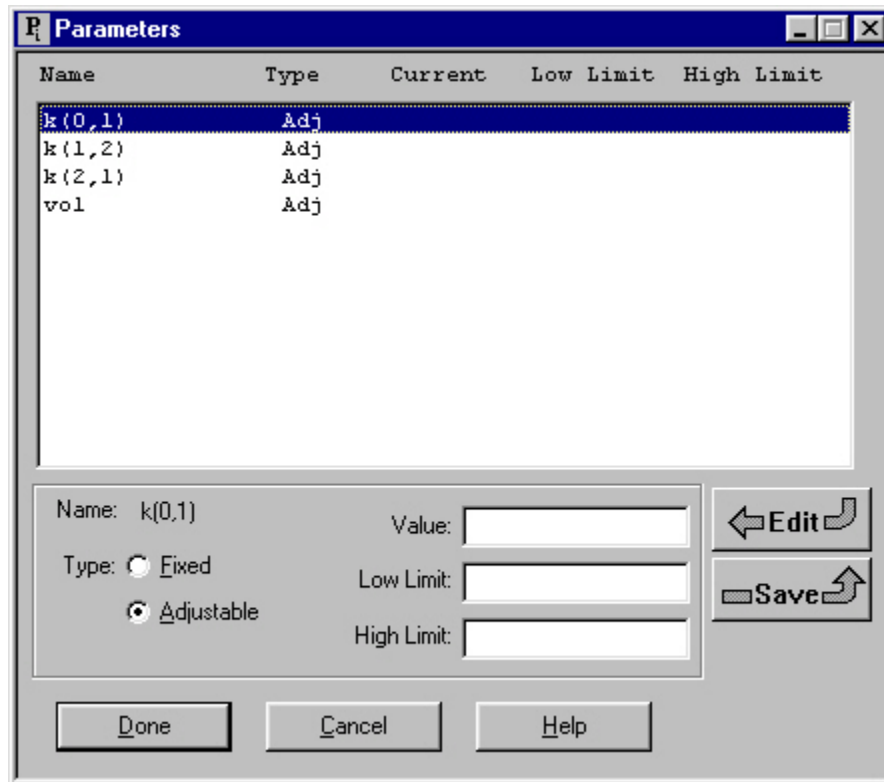
Error structure of the data. For this introductory tutorial, the errors in the data are assumed to be a constant coefficient of variation; in this case Fractional Standard Deviation (FSD); this is denoted in the data file by *(FSD 0.1)*.



- Enter the parameter values.

The parameters for the model are $k(2,1)$, $k(1,2)$, $k(0,1)$ and vol .

- a. In the **Show** menu, click **Parameters**, or alternatively, on the **SAAM II Toolbar** click **Parameters** . The **Parameters** dialog box will open as follows:



The parameter $k(0,1)$ should be selected. If it is not selected, double-click $k(0,1)$ to select it. Be sure the **Adjustable** button is selected.

- b. Enter "0.1" in the **Value** box, and click **Save**.



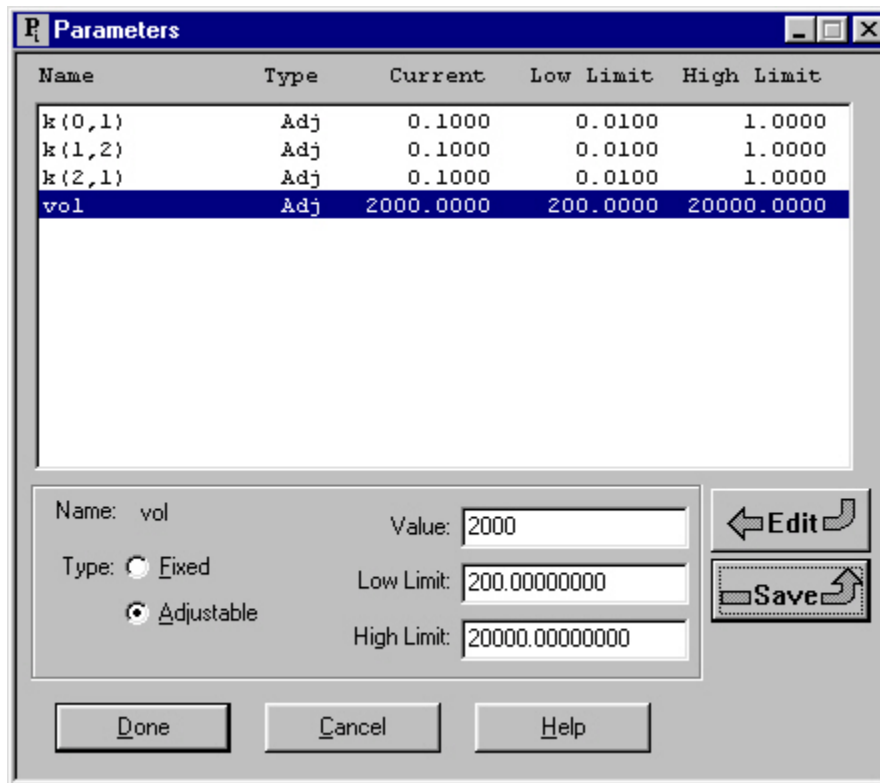
Default low and high parameter limits. Notice that when a value is entered in the **Value** box and nothing is entered in the **Low Limit** or **High Limit** boxes, the default low and high limits of one tenth of the value and ten times the value respectively are automatically entered when the value is saved.



- c. Double-click $k(1,2)$ to select it.
- d. Enter "0.1" in the **Value** box, and click **Save**.
- e. Double-click $k(2,1)$ to select it.

- f. Enter "0.1" in the **Value** box, and click **Save**.
- g. Double-click *vol* to select it.
- h. Enter "2000" in the **Value** box, and click **Save**.

When you have finished, the **Parameters** dialog box should appear as follows:



- i. Click **Done**.



*Single or double-clicking a parameter in the **Parameters** dialog box.* When the **Parameters** dialog box is open, there is always a current parameter. Its name appears in **Name:** in the lower pane. The **Value**, **Low Limit** and **High Limit** boxes will either contain the values associated with the current parameter or be empty if no values have been entered.

If you single-click on another parameter, the **Name** of the current parameter will not change nor will the entries in the **Value**, **Low Limit** and **High Limit** boxes. However, if you click **Save**, the current **Value**, **Low Limit** and **High Limit** shown in the boxes will be saved for the new parameter. This makes it easy to enter the same values for more than one parameter.

If you double-click on another parameter, the name of the new parameter will appear in **Name:**. The **Value**, **Low Limit** and **High Limit** boxes will change to the values associated with this parameter. If no values were entered for this parameter, these boxes will be cleared, and you can enter the new values for this parameter.



You have now successfully created the model used in Part 1 of the tutorial.

12. **Quit the SAAM II Compartmental application.**

- a. In the **File** menu, click **Exit**.
- b. Click **No**.

Data for this tutorial

```
DATA
(FSD 0.1)
t      plasma
0.007 46780
0.042 43522
0.125 42535
0.25  40125
0.375 36221
0.5   35562
1.0   28194
2.0   19573
3.0   14403
4.0   11278
5.0   8081
6.0   6999
7.0   5653
8.0   5139
9.0   4210
END
```