# SAAM II Version 2.2 Basic Tutorials

## Writing Reports

	Introduction	Reports – 1
Part 1	Using the Notes Window	Reports – 4
Part 2	Creating Text Files	Reports – 10

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.

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### Writing Reports

#### 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 create and save material to prepare reports. You will learn

- How to use the **Notes** window (Part 1)
- How to create and use text files (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.

#### SAAMII Version 2.1 Update:

- The export capabilities as well as copy & paste functions have been updated to allow for easier transfer of plots, data and results to other applications. In most menus including Data, Equations, Tables and Values, standard shortcuts such as "Ctrl + c" (copy) and "Ctrl + a" (select all) are available to quickly select, copy and paste information to other applications. "Ctrl + c" (copy) generally selects and copies all data in the window where your cursor rests.
- Notes Window: The user is encouraged to take advantage of the Notes window to track modeling setup and choices with your saved model. Accurate notes can document your model development and maintain a record with your saved model file.
- Save Results to Text File: Several settings are available as explained herein. Setting up the 'page setup' to landscape allows for a clearer view of tabular results in the saved text files. Copy information directly into other applications.

#### Introduction

This tutorial focuses on how to create material to prepare a report, and how to copy the material into other applications such as Microsoft Word®. All of the tutorials in the Using SAAM II series have been created using Microsoft Word® and by copying material created during a SAAM II modeling exercise into this application.

A variety of techniques can be used. One is to copy or export tabular information to a spreadsheet application such as Microsoft Excel® or Microsoft Word®. Another is to use the screen print capability or a software tool which will allow you to capture portions of your computer screen. These can be saved, and then copied into a Microsoft Word® document. All of these were used in creating the Using SAAM II tutorials.

The major options in SAAM II to create and save material for report writing are the **Notes** window, and saving information to a text file.

The **Notes** window is accessed from the **SAAM II Toolbar**. This will be explained in Part 1 of this tutorial.

In the **Compute** menu, select **Settings** to access the **Computational Settings** dialog box. *Saving information to a text file* is set up in the **Computational Settings** dialog box shown below:

Rosenbrock Pade Runge-Kutta	✓ Use Relative Error:     0.00100000     (1.0e-10 to 1.0)     Use Absolute Error:
Compute Sample AUC's	(greater than 0.0)
Variance Model © Data © Model Convergence Criterion	solute ative
Include Bayesian Term	(1.0e-7 to 1.0) (1.0e-7 to 1.0) (1.0e-7 to 1.0e7
Save Results to Text F	File C Replace C Add

Save Results to Tex	t File
C Basic C Detailed	C Replace

You can see the **Save Results to Text File** check box. When this box is selected, the options will appear as follows:

level	and the second second
Level	File
Basic	Replace     Replace
Detailed	C ALL

There are three levels of information that can be saved, **Basic**, **Detailed** and **All**; each will be illustrated in Part 2. In terms of creating the text file, you can **Replace** the existing saved file or **Add** to it. These options will also be explained in Part 2.

#### Part 1. Using the Notes Window

The **Notes** window can be used to create and retain information of interest for a given model, such as a description of what is being modeled, comments on certain aspects of the model, a description of sampling techniques, etc. The **Notes** window is a standard text window and accepts normal editing. The contents of the **Notes** window are automatically saved with the model when you save the model. The **Notes** window may be left open while you are working on other parts of the model.

This tutorial will show you have to save some material in the **Notes** window. What is illustrated is not exhaustive as you have many options.

- 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. The **Notes** window creating baseline information. (this information can be automatically saved by saving results to text file, append)
  - a. In the Show menu, click Notes, or alternatively, on the SAAM II Toolbar click
     Notes . The Notes window will open as shown below:



- b. Type "Work with study\_0 on January 1, 2011" as the first line of the **Notes** window.
- c. Solve the model. In the Compute menu, click Solve, or alternatively, on the SAAM II Toolbar, click Solve
- c. In the Show menu, click Values, or alternatively, on the SAAM II Toolbar click
   Values III. The Values window will open. Select the material as shown below:

📲 Values		
Values at t = $0$	0.0 days	Calculation Points:
ex1.bolus ex1.infusion flux(0,1) flux(1,2) flux(2,1) k(0,1)	1.040000e+008 0.000000 1.040000e+007 0.000000 1.040000e+007 0.100000	0.0000 0.0070 0.0420 0.1250 0.2500 0.3750 0.5000
k(1,2) k(2,1) plasma ql q2 sl sl res	0.100000 0.100000 - 1.040000e+008 0.000000 52000.000000 -	Variables Included: Variables Included: ex1.bolus ex1.infusion flux(0,1) flux(1,2) (lux(2,1))
sl_wres t vol	- 0.000000 2000.000000	K(0.1) k(1.2) Mode
		▼

- d. In the **Edit** menu, click **Copy**. You may also Right-Click and select Copy or simply type "Ctrl + c". Close the **Values** window.
- e. In the Notes window, line down and type "Baseline Solution".
- f. In the **Edit** menu, click **Paste** or "Ctrl + v". The **Notes** window will appear as follows:

Notes		
Work with study	y_0 on January 1, 2011	-
Baseline Solutio	n	
alues at $t = 0.0$	minutes	
ex1.bolus	1.040000e+008	
ex1.infusion	0.000000	
flux(0,1)	1.040000e+007	
flux(1,2)	0.000000	
flux(2,1)	1.040000e+007	
k(0,1)	0.100000	
k(1,2)	0.100000	
k(2,1)	0.100000	
plasma	-	
q1	1.040000e+008	
g2	0.000000	
s1	52000.000000	
s1 res	and the set of the set	
s1 wres		
t	0.000000	
vol	2000.000000	
		<u></u>

Your **Notes** window now contains information about the baseline solution, i.e. the solution with the set of parameter values indicated, and the bolus injection also as indicated. Notice the initial value for **q1** equals **ex1.bolus**; this is because "q1(0) = ex1.bolus", i.e. the initial conditions for q1(t) are **ex1.bolus**. Similarly at time zero, q2(0) = 0 since there is no initial input into **q2**. There is no data "plasma" at time zero since there was no measured value at time zero. Finally, there are no values for **s1\_res** or **s1\_wres** since the model has not been fitted to the data.

Leave the Notes window open.



*Using Notes.* You can record information about all your modeling activities in the Notes window. If you were to hand-fit the model to the data, you can record the values following each change in parameter values. You can copy information from the **Table** window into the **Notes** window. You cannot copy a plot into the **Notes** window.



- 5. The Notes window saving information following a fit.
  - a. Fit the model to your data. In the **Compute** menu, click **Fit**, or alternatively, on the **SAAM II Toolbar** click **Fit**.
  - b. In the Notes window, type "Results following a Fit".
  - c. In the Show menu, click Statistics, or alternatively on the SAAM II Toolbar click
     Statistics Statistics window will open.
  - d. Select and copy the material in the top pane of the **Statistics** window. The **Statistics** window will appear as follows:

arameter/Variable	Value	Std.Dev.	Coef. of Var.	95% Confiden	ce 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	
C Correlation Matrix	C Covariance M	atrix 🕞	Objective Scaled Data Va	ariance		
C Correlation Matrix	Covariance M Obj 1.336743e+	atrix 💽 ective 001	Objective Scaled Data V 1.113515e-002	ariance 1		
C Correlation Matrix s1 : plasma Total objective	C Covariance M Obj 1.336743e+ 1.336743e+	ective 001 	Objective Scaled Data Va 1.113515e-00:	ariance 1		
C Correlation Matrix s1 : plasma Total objective AIC	C Covariance M Obj 1.336743e+ 	atrix •	Objective Scaled Data Va 1.113515e-00:	ariance 1		
C Correlation Matrix s1 : plasma Total objective AIC BIC	C Covariance M Obj 1.336743e+ 1.336743e+ 7.935987e+ 8.053995e+	atrix (* ective 	Objective Scaled Data Va 1.113515e-00:	ariance 1		

- e. Return to the **Notes** window. Right-click in the **Notes** window and select **Paste**, or in the **Edit** menu, click **Paste**. The copied material will appear in the **Notes** window. It is not possible to copy the labels of each column, so you will have to type them in yourself (as shown below).
- f. Return to the **Statistics** window, select and copy the information in the bottom page.
- g. Return to the **Notes** window. In the **Edit** menu, click **Paste**. The **Notes** window will appear as follows:

```
Notes
                                                                                                                                                                  <u>- 🗆 ×</u>
 Work with study_0 on January 1, 2003
                                                                                                                                                                           ۰
Baseline solution
 Values at t = 0.0 days
                                         1.040000e+008
 exl.bolus
 ex1.infusion 0.000000
flux(0,1) 1.0400000
 flux(0,1)
                                         1.040000e+007
0.000000
 flux(1,2)
                                        1.040000e+007
 flux(2,1)
k(0,1)
                                        0.100000
k(1,2)
                                          0.100000
                                        0.100000
k(2,1)
plasma
                                              _
 ql
                                        1.040000e+008
                                0.000000
 q2
 sl
 sl_res
                                            -
 sl_wres
                                             _
                                          0.000000
 t
 vol
                                     2000.000000
 Results following a Fit

        Value
        SD
        Coeff Var
        95% Confidence

        0.29227
        1.46155e-002
        5.00071e+000
        0.26010
        0.32444

        0.28311
        7.51183e-002
        2.65335e+001
        0.11777
        0.44844

        0.17452
        1.82636e-002
        1.04652e+001
        0.13432
        0.21472

      Parameter
      k(0,1)
      0.29227
      1.461335
      0.2

      k(1,2)
      0.28311
      7.51183e-002
      2.65335e+001
      0.2

      k(2,1)
      0.17452
      1.82636e-002
      1.04652e+001
      0.13432
      0.21472

      wol
      2323.77661
      3.85619e+001
      1.65945e+000
      2238.90219
      2408.65103

 Parameter
 sl : plasma
                                            _____
 Total objective
                                           1.336743e+001
                                             7.935987e+000
 AIC
 BIC
                                              8.053995e+000
```

h. Close the Notes window.

Quit the SAAM II Compartmental application. Do not save the changes to study\_0.

The **Notes** window acts like a note pad. It is a text file into which you can type your own notes and paste information generated during your SAAM II modeling session. If you were to save your study file, your notes will be saved so the next time you open the study file, the notes will be there.

You can also copy the contents of your **Notes** window into other applications such as Microsoft Word®. Notes are very flexible and helpful for keeping track of your modeling activities.

#### Part 2. Creating Text Files

SAAM II has the option of creating text files every time you Solve or Fit. There are three levels of information, Basic, Detailed and All. A quick summary of the type of information contained in each report is shown below. The reports will be explained in this tutorial since the level of information you need to write your report may vary depending upon the type of report you are preparing.

SAAM II Save Re	SAAM II Save Results Options					
Information Type	Basic	Detailed	All			
Study Information	Х	X	Х			
Computational Settings	X	X	Х			
Experimental Attributes		X	Х			
Model Equations			Х			
Data			Х			
Exogenous Inputs			Х			
Change Conditions			Х			
General Model Information			Х			
Parameter Values		X	Х			
Values at t=0.0	Х	X	Х			
Calculated Samples and Data	X	X	Х			
Statistics	Х	X	Х			
Notes		X	Х			

You also have the option of over writing the text file after each Solve or Fit; this is helpful if you are concerned about using a lot of space, and don't need the intermediate information. Alternatively, you can create a new file after each Solve or Fit; they are named in such a way that you can follow what you did sequentially.

- 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. Turning on the Save Results option.
  - a. In the **Compute** menu, click **Settings**. The **Computational Settings** dialog box will open as shown below:

Computational Settings	? ×
Min. Nr. of Calculations Intervals: 🔽 💌 (1 to	500)
Integrator Rosenbrock Pade Runge-Kutta Use Relative Error: 0.00100000 (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  C Data C Absolute C Model C Relative C Central	ł
Convergence Criterion: 0.00010000 (1.0e-7 to 1.0) Include Bayesian Term Lambda: 10.00000000 (1.0e-7 to 1.0e	:7)
Save Results to Text File  Level  C Basic  Detailed  C All	
Done Cancel Help	

The bottom pane of the dialog box contains the **Save Results to Text File** check box. If this box is checked, the **Level** and **File** panes become active.

b. Select Save Results to Text File. The pane will appear as follows:

Level	File
Basic	Replace
Detailed	C Add

The default settings are Basic-Replace meaning just the basic information is written to the file, and the file is replaced if you do another Solve or Fit.

#### c. Click Done.

5. Solve the model, and view the text file created.

- a. In the **Compute** menu, click **Solve**, or alternatively, on the **SAAM II Toolbar**, click **Solve**
- b. Go to the folder where **study\_0** is located. In this folder, you will find a file entitled **study\_0.txt**. The contents of this file are shown below:

Study Name: study 0.stu Basic Summary Output Date: 07:29 AM, Tuesday, January 18, 2011 Application: Compartmental Type of Calculation: Solve \_\_\_\_\_ Computational Settings Integrator: Rosenbrock Relative Integrator Error: 1.0000e-003 \_\_\_\_\_ Values at t = 0.0 days 

 ex1.bolus
 1.040000e+000

 ex1.infusion
 0.000000

 flux(0,1)
 1.040000e+007

 0.000000
 0.000000

 flux(2,1) 1.040000e+007 0.100000 k(0,1) 0.100000 k(1,2) 0.100000 k(2,1) plasma \_ 1.040000e+008 ql 0.000000 q2 52000.000000 s1 sl res -\_ sl wres 0.00000 t 2000.000000 vol \_\_\_\_\_ \_\_\_\_\_

Calculated Sample Values and Data

t	plasma	Weight	s1	s1 wres
0.000e+000		_	5.200e+004	
7.000e-003	4.678e+004	-	5.193e+004	-
4.200e-002	4.352e+004	-	5.157e+004	-
1.250e-001	4.254e+004	-	5.072e+004	-
2.500e-001	4.013e+004	-	4.948e+004	-
3.750e-001	3.622e+004	-	4.828e+004	-
5.000e-001	3.556e+004	-	4.711e+004	-
7.500e-001	-	-	4.489e+004	-
1.000e+000	2.819e+004	-	4.279e+004	-
1.450e+000	-	-	3.934e+004	-
1.725e+000	-	-	3.741e+004	-
2.000e+000	1.957e+004	-	3.561e+004	-
2.450e+000	-	-	3.290e+004	-

2.725e+000	-	_	3.139e+004	_
3.000e+000	1.440e+004	-	2.997e+004	-
3.450e+000	-	_	2.785e+004	-
3.725e+000	-	-	2.666e+004	-
4.000e+000	1.128e+004	-	2.554e+004	-
4.450e+000	-	-	2.386e+004	-
4.725e+000	-	-	2.292e+004	-
5.000e+000	8.081e+003	-	2.204e+004	-
5.450e+000	-	-	2.070e+004	-
5.725e+000	-	-	1.996e+004	-
6.000e+000	6.999e+003	-	1.925e+004	-
6.450e+000	-	-	1.819e+004	-
6.725e+000	-	-	1.759e+004	-
7.000e+000	5.653e+003	-	1.702e+004	-
7.450e+000	-	-	1.616e+004	-
7.725e+000	-	-	1.568e+004	-
8.000e+000	5.139e+003	-	1.522e+004	-
8.450e+000	-	-	1.453e+004	-
8.725e+000	-	-	1.413e+004	-
9.000e+000	-	-	1.376e+004	-
9.000e+000	4.210e+003	-	1.376e+004	-

Statistics

No Statistics after a Solve

The first line of the file is simply the name of the study file. The next is the type of output, in this case, Basic. Next is the date followed by the SAAM II Application, in this case, Compartmental. Finally, the type of calculation which produced the output is given, in this case, Solve.

The Computational settings provide the chosen integrator and the setting for the Relative Integrator Error.

This is followed by the values at time zero. This information is the same as that in the **Values** window at time zero.

The calculated sample values and data come next in a table. Notice the weights or weighted residuals are not given; this is because the calculation was a Solve and not a Fit.

Values for **s1** are given at all calculation points; this is why there are more **s1** values here than for data. Remember the number of calculation points is set in the **Computational Settings** dialog box in the **Min. Nr. Calculation Intervals** box.

This information can be cut from the text window and pasted into another application for you to prepare your report.

c. Close the text file and return to **study\_0**.

- 6. Fit the model, and view the text file created.
  - a. In the **Compute** menu, click **Fit**, or alternatively, on the **SAAM II Toolbar** click **Fit**
  - b. Go to the folder where study\_0 is located. In this folder, you will find the file study\_0.txt. This file contains the following information (note the previous file has been over written):

```
Study Name: study 0.stu
Basic Summary Output
Date: 02:40 PM, Tuesday, January 17, 2011
Application: Compartmental
Type of Calculation: Fit
      _____
Computational Settings
Integrator: Rosenbrock
Relative Integrator Error: 1.0000e-003
Variance Model: Data, Relative
Derivative: Forward
_____
Values at t = 0.0 days
ex1.bolus
                 1.040000e+008
ex1.infusion flux(0,1)
                0.00000
                 3.039597e+007
                 0.00000
flux(1,2)
flux(2,1)
                 1.814980e+007
k(0,1)
                 0.292269
k(1,2)
                 0.283108
                 0.174517
k(2,1)
plasma
                  _
                 1.040000e+008
q1
                 0.000000
q2
              44754.732253
s1
sl res
                  -
sl wres
                   _
t
                 0.000000
vol
               2323.776610
```

Calculated Sample Values and Data

t	plasma	Weight	sl	s1 wres
0.000e+000	-	-	4.475e+004	_
7.000e-003	4.678e+004	4.104e-007	4.461e+004	1.391e+000
4.200e-002	4.352e+004	4.741e-007	4.389e+004	-2.519e-001
1.250e-001	4.254e+004	4.964e-007	4.223e+004	2.117e-001
2.500e-001	4.013e+004	5.578e-007	3.989e+004	1.772e-001

3.750e-001	3.622e+004	6.845e-007	3.770e+004	-1.225e+000	
5.000e-001	3.556e+004	7.101e-007	3.566e+004	-8.650e-002	
7.500e-001	-	-	3.200e+004	-	
1.000e+000	2.819e+004	1.130e-006	2.880e+004	-6.469e-001	
1.450e+000	-	-	2.405e+004	-	
1.725e+000	-	-	2.166e+004	-	
2.000e+000	1.957e+004	2.344e-006	1.960e+004	-4.317e-002	
2.450e+000	-	-	1.680e+004	-	
2.725e+000	-	-	1.537e+004	-	
3.000e+000	1.440e+004	4.329e-006	1.412e+004	5.867e-001	
3.450e+000	-	-	1.240e+004	-	
3.725e+000	-	-	1.151e+004	-	
4.000e+000	1.128e+004	7.061e-006	1.072e+004	1.494e+000	
4.450e+000	-	-	9.603e+003	-	
4.725e+000	-	-	9.016e+003	-	
5.000e+000	8.081e+003	1.375e-005	8.487e+003	-1.507e+000	
5.450e+000	-	-	7.728e+003	-	
5.725e+000	-	-	7.319e+003	-	
6.000e+000	6.999e+003	1.833e-005	6.944e+003	2.355e-001	
6.450e+000	-	-	6.395e+003	-	
6.725e+000	-	-	6.093e+003	-	
7.000e+000	5.653e+003	2.810e-005	5.813e+003	-8.504e-001	
7.450e+000	-	-	5.396e+003	-	
7.725e+000	-	-	5.162e+003	-	
8.000e+000	5.139e+003	3.401e-005	4.943e+003	1.142e+000	
8.450e+000	-	-	4.612e+003	-	
8.725e+000	-	-	4.424e+003	-	
9.000e+000	-	-	4.246e+003	-	
9.000e+000	4.210e+003	5.067e-005	4.246e+003	-2.582e-001	

Statistics

Parameter/Variable	Value	Std.Dev.	Coef. of Var.	95% Confidenc	e 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

Obj	ective s1 : plasma	Scaled Data	Variance 1.336743e+001	1	.113515e-001	L
	Total object	tive	1.336743e+001			
	AIC BIC		7.935987e+000 8.053995e+000			
	Number of It	terations Rec	quired to Fit: 5	5		

This contains the same information as that following a Solve except information about the Fit and statistics is available.

c. Close **study\_0.txt**, and return to **study\_0.stu**.

Quit the SAAM II Compartmental application. Do not save the changes to study\_0.

You will now repeat what you did above, only observe the **Detailed** output and set the **File** option to **Add**.

- 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:



- 4. Turning on the Save Results option.
  - a. In the **Compute** menu, click **Settings**. The **Computational Settings** dialog box will open as shown below:

Computational Settings
Min. Nr. of Calculations Intervals: (1 to 500) Integrator Rosenbrock 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 O Absolute O Data O Absolute O Model O Central
Convergence Criterion: 0.00010000 (1.0e-7 to 1.0) Include Bayesian Term Lambda: 10.0000000 (1.0e-7 to 1.0e7)
Level File C Replace C Detailed All Cancel Help

The bottom pane of the dialog box contains the **Save Results to Text File** check box. If this box is checked, the **Level** and **File** panes become active.

b. Select **Save Results to Text File**. In the **Level** pane, select **Detailed**. In the **File** pane, select **Add**. The panes will appear as follows.

Save Results to Te	xt File
C Basic C Basic C Detailed C All	C Replace C Add

- c. Click **Done**. You will now produce more detailed information, and will produce a file each time you Solve or Fit.
- 5. Solve the model, and view the text file created.
  - a. In the **Compute** menu, click **Solve**, or alternatively, on the **SAAM II Toolbar**, click **Solve**
  - b. Go to the folder where **study\_0** is located. In this folder, you will find a file entitled **study\_0.txt**. The contents of this file are shown below:

```
Study Name: study 0.stu
Detailed Summary Output
Date: 07:36 AM, Tuesday, January 17, 2011
Application: Compartmental
Type of Calculation: Solve
_____
Computational Settings
Number of Calculation Intervals: 20
Integrator: Rosenbrock
Relative Integrator Error: 1.0000e-003
Maximum Number of Iterations: 20
_____
                        _____
Experiment Attributes
Independent Variable: t (days)
Start of Experiment: 0.0000e+000
End of Experiment: 9.0000e+000
   _____
Parameter Values
Parameter Type Prior Value New Value Lower Limit Upper Limit
                                            __ _____
k(0,1)
       Adj 1.000e-001 1.000e-001 1.000e-002 1.000e+000
k(1,2)
       Adj 1.000e-001 1.000e-001 1.000e-002 1.000e+000
k(2,1)
       Adj 1.000e-001 1.000e-001 1.000e-002 1.000e+000
vol
      Adj 2.000e+003 2.000e+003 2.000e+002 2.000e+004
```

Values at t = 0.0 days

ex1.bolus	1.040000e+008	
ex1.infusion	0.00000	
flux(0,1)	1.040000e+007	
flux(1,2)	0.00000	
flux(2,1)	1.040000e+007	
k(0,1)	0.100000	
k(1,2)	0.100000	
k(2,1)	0.100000	
plasma	-	
q1	1.040000e+008	
q2	0.00000	
s1	52000.000000	
s1_res	-	
s1_wres	-	
t	0.00000	
vol	2000.000000	

Calculated Sample Values and Data

t	plasma	Weight	s1	s1_wres
0.000e+000	-	-	5.200e+004	_
7.000e-003	4.678e+004	-	5.193e+004	-
4.200e-002	4.352e+004	-	5.157e+004	-
1.250e-001	4.254e+004	-	5.072e+004	-
2.500e-001	4.013e+004	-	4.948e+004	_
3.750e-001	3.622e+004	-	4.828e+004	_
5.000e-001	3.556e+004	-	4.711e+004	_
7.500e-001	-	-	4.489e+004	-
1.000e+000	2.819e+004	-	4.279e+004	_
1.450e+000	-	-	3.934e+004	_
1.725e+000	-	-	3.741e+004	_
2.000e+000	1.957e+004	-	3.561e+004	_
2.450e+000	-	-	3.290e+004	_
2.725e+000	-	-	3.139e+004	_
3.000e+000	1.440e+004	-	2.997e+004	_
3.450e+000	-	-	2.785e+004	_
3.725e+000	-	-	2.666e+004	_
4.000e+000	1.128e+004	-	2.554e+004	_
4.450e+000	-	-	2.386e+004	_
4.725e+000	-	-	2.292e+004	_
5.000e+000	8.081e+003	-	2.204e+004	_
5.450e+000	-	-	2.070e+004	_
5.725e+000	-	-	1.996e+004	-
6.000e+000	6.999e+003	-	1.925e+004	-
6.450e+000	-	-	1.819e+004	-
6.725e+000	-	-	1.759e+004	-
7.000e+000	5.653e+003	-	1.702e+004	-
7.450e+000	-	-	1.616e+004	-
7.725e+000	-	-	1.568e+004	-
8.000e+000	5.139e+003	-	1.522e+004	-
8.450e+000	-	-	1.453e+004	-
8.725e+000	-	-	1.413e+004	_
9.000e+000	-	-	1.376e+004	-
9.000e+000	4.210e+003	-	1.376e+004	_

```
Statistics
No Statistics after a Solve
Notes
None
```

This file contains all of the information contained in the "Basic" option plus additional information. There is more information about the Computational Settings. The file contains the Experimental Attributes and the initial parameter values. Finally, at the very end, are the contents of the **Notes** window. In this case there are no notes. If you have information in the **Notes** window, it would appear here.

- c. Close the text file, and return to **study\_0**.
- 6. Fit the model, and view the text file created.
  - a. In the **Compute** menu, click **Fit**, or alternatively, on the **SAAM II Toolbar** click **Fit**
  - b. Go to the folder where **study\_0** is located. In this folder, you will find a file entitled **study\_0.txt**. and **study\_0\_01.txt**



The file **study\_0\_01** contains the information following the Fit. Each time you solve or fit, you will produce a file with a number such as "01" after it. If you are doing this several times, it is useful to keep track of the number using Notes.

The contents of **study\_0\_01** are shown below.

Derivative: Forward

Experiment Attributes

Independent Variable: t (days) Start of Experiment: 0.0000e+000 End of Experiment: 9.0000e+000

Parameter Values

Parameter Type Prior Value New Value Lower Limit Upper Limit

k(0,1)	Adj 1.000e-001 2.923e-001 1.000e-002 1.000e+000	
k(1,2)	Adj 1.000e-001 2.831e-001 1.000e-002 1.000e+000	
k(2,1)	Adj 1.000e-001 1.745e-001 1.000e-002 1.000e+000	
vol	Adj 2.000e+003 2.324e+003 2.000e+002 2.000e+004	

Values at t = 0.0 days

ex1.bolus	1.040000e+008	
ex1.infusion	0.00000	
flux(0,1)	3.039597e+007	
flux(1,2)	0.00000	
flux(2,1)	1.814980e+007	
k(0,1)	0.292269	
k(1,2)	0.283108	
k(2,1)	0.174517	
plasma	-	
q1	1.040000e+008	
q2	0.00000	
s1	44754.732253	
sl res	-	
s1 wres	-	
t –	0.00000	
vol	2323.776610	

Calculated Sample Values and Data

t	plasma	Weight	s1	s1 wres
0.000e+000	-	-	4.475e+004	_
7.000e-003	4.678e+004	4.104e-007	4.461e+004	1.391e+000
4.200e-002	4.352e+004	4.741e-007	4.389e+004	-2.519e-001
1.250e-001	4.254e+004	4.964e-007	4.223e+004	2.117e-001
2.500e-001	4.013e+004	5.578e-007	3.989e+004	1.772e-001
3.750e-001	3.622e+004	6.845e-007	3.770e+004	-1.225e+000
5.000e-001	3.556e+004	7.101e-007	3.566e+004	-8.650e-002
7.500e-001	-	-	3.200e+004	-
1.000e+000	2.819e+004	1.130e-006	2.880e+004	-6.469e-001
1.450e+000	-	-	2.405e+004	-
1.725e+000	-	-	2.166e+004	-
2.000e+000	1.957e+004	2.344e-006	1.960e+004	-4.317e-002
2.450e+000	-	-	1.680e+004	-
2.725e+000	-	-	1.537e+004	-
3.000e+000	1.440e+004	4.329e-006	1.412e+004	5.867e-001

3.450e+000 3.725e+000 4.000e+000 4.450e+000 5.000e+000 5.450e+000 5.725e+000 6.000e+000 6.450e+000 6.725e+000 7.000e+000 7.450e+000 8.000e+000 8.450e+000	- - 1.128e+004 - - 8.081e+003 - - 6.999e+003 - - 5.653e+003 - - 5.139e+003 -	- 7.061e-006 - - 1.375e-005 - - 1.833e-005 - - 2.810e-005 - - 3.401e-005	1.240e+004 1.151e+004 1.072e+004 9.603e+003 9.016e+003 8.487e+003 7.728e+003 6.944e+003 6.994e+003 6.093e+003 5.813e+003 5.396e+003 5.162e+003 4.943e+003 4.612e+003	- 1.494e+000 - -1.507e+000 - 2.355e-001 - - -8.504e-001 - 1.142e+000 -	
8.000e+000 8.450e+000	5.139e+003 -	3.401e-005 -	4.943e+003 4.612e+003	1.142e+000 _	
8.725e+000 9.000e+000			4.424e+003 4.246e+003	-	
9.000e+000	4.210e+003	5.067e-005	4.246e+003	-2.582e-001	

#### Statistics

Parameter/Variable V	Value Std.Dev. Co	oef. of Var.	95% Confider	nce Interval
k(0,1)         0.29227           k(1,2)         0.28311           k(2,1)         0.17452           vol         2323.77661	1.46155e-002 5.00 7.51183e-002 2.65 1.82636e-002 1.04 3.85619e+001 1.6	0071e+000 5335e+001 4652e+001 65945e+000	0.26010 0.11777 0.13432 2238.90219	0.32444 0.44844 0.21472 2408.65103
s1 : plasma	Objecti 1.336743e	ive S e+001	caled Data 1.113515e	Variance e-001
Total objective	1.336743e	e+001		
AIC BIC	7.935987e 8.053995e	e+000 e+000		
Number of Iteratio	ns Required to	Fit: 5		
Notes				
None				

The information parallels that following the Solve except now information on the Fit is available. This includes the weights and weighted residuals, and the information from the **Statistics** window. It also includes the number of iterations required to Fit the data.

If you had information in the Notes window, it would appear at the end of this file.

c. Close the text file, and return to **study\_0.stu**.

This information can be cut from the text window and pasted into another application for you to prepare your report.

Quit the SAAM II Compartmental application. Do not save the changes to study\_0.

You will now repeat what you did above, only select the **All** output and set the **File** option to **Add**.

- 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:



- 4. Turning on the Save Results option.
  - a. In the **Compute** menu, click **Settings**. The **Computational Settings** dialog box will open as shown below:

Computational Settings	<u>? ×</u>
Min. Nr. of Calculations Intervals: 🗾 💌 (1 to	500)
Integrator Use Relative Error:	
Pade 0.00 100000	
Runge-Kutta (1.0e-10 to 1.0)	
I Use Absolute Error:	
Compute Sample AUC's (greater than 0.0)	
Optimizer	
Data     O     Absolute     O     Eorward	
C Model    Relative  C Central	1
Convergence Criterion: 0.00010000 (1.0e-7 to 1.0)	
Include Bayesian Term	
Lambda: 10.0000000 (1.0e-7 to 1.0e	:7)
Save Results to Text File	
C Basic	
C Detailed C Add	
Done Cancel Help	

The bottom pane of the dialog box contains the **Save Results to Text File** check box. If this box is checked, the **Level** and **File** panes become active.

b. Select **Save Results to Text File**. In the **Level** pane, select **All**. In the **File** pane, select **Add**.

Save Results to Te	xt File
C Basic	File
C Detailed	C Replace
C All	C Add

- c. Click **Done**. You will now produce more detailed information, and will produce a file **each time you Solve or Fit**.
- 5. Solve the model, and view the text file created.
  - a. In the **Compute** menu, click **Solve**, or alternatively, on the **SAAM II Toolbar**, click **Solve**

b. Go to the folder where **study\_0** is located. In this folder, you will find a file entitled study\_0.txt. The contents of this file are shown below:

```
Study Name: study 0.stu
Model and Detailed Summary Output
Date: 08:08 AM, Tuesday, January 17, 2011
Application: Compartmental
Type of Calculation: Solve
_____
Computational Settings
Number of Calculation Intervals: 20
Integrator: Rosenbrock
Relative Integrator Error: 1.0000e-003
Maximum Number of Iterations: 20
_____
                          _____
Experiment Attributes
Independent Variable: t (days)
Start of Experiment: 0.0000e+000
End of Experiment: 9.0000e+000
_____
Model Equations
flux(1,2) = k(1,2) * q2
flux(2,1) = k(2,1) * q1
flux(0,1) = k(0,1) * q1
ex1.bolus = 0.0
ex1.infusion = 0.0
s1 = q1/vol
q1' = + k(1,2)*q2 - k(2,1)*q1 - k(0,1)*q1 + ex1
q2' = -k(1,2)*q2 + k(2,1)*q1
_____
                    _____
Data
DATA
t plasma
```

```
(FSD 0.1)
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 \_\_\_\_\_ Exogenous Inputs Name: ex1 Experiment: tracer Input to: q1 Type Input Constant Start Stop Interval Number \_\_\_\_\_ \_\_\_\_ Bolus 1.0400e+008 \_ 0.0000e+000 \_\_\_\_\_ Change Conditions No Change Conditions \_\_\_\_\_ General Model Information Compartment Numbers in Model: 1, 2 No Delays Experiments: Name Туре Suffix ----- -----\_ tracer Exogenous \_\_\_\_\_ \_\_\_\_\_ Parameter Values Parameter Type Prior Value New Value Lower Limit Upper Limit k(0,1) Adj 1.000e-001 1.000e-001 1.000e-002 1.000e+000 Adj 1.000e-001 1.000e-001 1.000e-002 1.000e+000 k(1,2) k(2,1) Adj 1.000e-001 1.000e-001 1.000e-002 1.000e+000 Adj 2.000e+003 2.000e+003 2.000e+002 2.000e+004 vol \_\_\_\_\_ Values at t = 0.0 days ex1.bolus 1.040000e+008 ex1.infusion 0.00000 1.040000e+007 flux(0,1) flux(1,2) 0.000000 flux(2,1) 1.040000e+007 k(0,1) 0.100000 0.100000 k(1,2) k(2,1) 0.100000 plasma 1.040000e+008 q1

0.000000

q2

s1	52000.000000		
s1 res	-		
s1 wres	-		
t –	0.00000		
vol	2000.000000		

Calculated Sample Values and Data

t	plasma	Weight	sl	s1 wres
0.000e+000		_	5.200e+004	_
7.000e-003	4.678e+004	-	5.193e+004	-
4.200e-002	4.352e+004	-	5.157e+004	_
1.250e-001	4.254e+004	-	5.072e+004	_
2.500e-001	4.013e+004	-	4.948e+004	_
3.750e-001	3.622e+004	-	4.828e+004	_
5.000e-001	3.556e+004	-	4.711e+004	-
7.500e-001	-	-	4.489e+004	-
1.000e+000	2.819e+004	-	4.279e+004	-
1.450e+000	-	-	3.934e+004	_
1.725e+000	-	-	3.741e+004	_
2.000e+000	1.957e+004	-	3.561e+004	-
2.450e+000	-	-	3.290e+004	-
2.725e+000	-	-	3.139e+004	_
3.000e+000	1.440e+004	-	2.997e+004	_
3.450e+000	-	-	2.785e+004	_
3.725e+000	-	-	2.666e+004	-
4.000e+000	1.128e+004	-	2.554e+004	-
4.450e+000	-	-	2.386e+004	-
4.725e+000	-	-	2.292e+004	-
5.000e+000	8.081e+003	-	2.204e+004	-
5.450e+000	-	-	2.070e+004	-
5.725e+000	-	-	1.996e+004	-
6.000e+000	6.999e+003	-	1.925e+004	-
6.450e+000	-	-	1.819e+004	-
6.725e+000	-	-	1.759e+004	-
7.000e+000	5.653e+003	-	1.702e+004	-
7.450e+000	-	-	1.616e+004	-
7.725e+000	-	-	1.568e+004	-
8.000e+000	5.139e+003	-	1.522e+004	-
8.450e+000	-	-	1.453e+004	-
8.725e+000	-	-	1.413e+004	-
9.000e+000	-	-	1.376e+004	-
9.000e+000	4.210e+003	-	1.376e+004	-
Statistics				
No Statistics	after a Solve	9		

Notes

None

This file contains all of the information contained in the "Detailed" option plus additional information. The model equations (that appear in the **Equations Read**-

**Only** window) are included. The data are also included as is information about the input and model (number of compartments).

- c. Close the text file, and return to **study\_0**.
- 6. Fit the model, and view the text file created.
  - a. In the **Compute** menu, click **Fit**, or alternatively, on the **SAAM II Toolbar** click **Fit**
  - b. Go to the folder where **study\_0** is located. In this folder, you will find a file entitled **study\_0.txt**. and **study\_0\_01.txt**



The file **study\_0\_01** contains the information following the Fit. Each time you solve or fit, you will produce a file with a number such as "01" after it. If you are doing this several times, it is useful to keep track of the number using Notes.

The contents of **study\_0\_01** are shown below.

```
Study Name: study 0.stu
Model and Detailed Summary Output
Date: 08:08 AM, Tuesday, January 17, 2011
Application: Compartmental
Type of Calculation: Fit
_____
Computational Settings
Number of Calculation Intervals: 20
Integrator: Rosenbrock
Relative Integrator Error: 1.0000e-003
Maximum Number of Iterations: 20
Variance Model: Data, Relative
Derivative: Forward
_____
Experiment Attributes
Independent Variable: t (days)
Start of Experiment: 0.0000e+000
End of Experiment: 9.0000e+000
                          _____
```

Model Equations

```
flux(1,2) = k(1,2) * q2
flux(2,1) = k(2,1) * q1
flux(0,1) = k(0,1) * q1
ex1.bolus = 0.0
ex1.infusion = 0.0
s1 = q1/vol
q1' = + k(1,2) * q2 - k(2,1) * q1 - k(0,1) * q1 + ex1
q2' = -k(1,2)*q2 + k(2,1)*q1
_____
                  _____
Data
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
_____
Exogenous Inputs
Name: ex1
Experiment: tracer
Input to: q1
Туре
        Input Constant Start Stop Interval
Number
_____ ____
     1.0400e+008
                 - 0.0000e+000
Bolus
                                     _
         _____
Change Conditions
No Change Conditions
             _____
General Model Information
Compartment Numbers in Model: 1, 2
No Delays
```

Experiments:

Name	Туре	Suffix
tracer	Exogenous	

#### Parameter Values

Parameter	Type Prior Value New Value Lower Limit Upper Limit	
k(0,1) k(1,2) k(2,1) vol	Adj       1.000e-001       2.923e-001       1.000e-002       1.000e+000         Adj       1.000e-001       2.831e-001       1.000e-002       1.000e+000         Adj       1.000e-001       1.745e-001       1.000e-002       1.000e+000         Adj       2.000e+003       2.324e+003       2.000e+002       2.000e+004	

Values at t = 0.0 days

vol	2323.776610	
t	0.00000	
s1_wres	-	
s1_res	-	
s1	44754.732253	
q2	0.00000	
q1	1.040000e+008	
plasma	-	
k(2,1)	0.174517	
k(1,2)	0.283108	
k(0,1)	0.292269	
flux(2,1)	1.814980e+007	
flux(1,2)	0.00000	
flux(0,1)	3.039597e+007	
ex1.infusion	0.00000	
ex1.bolus	1.040000e+008	

Calculated Sample Values and Data

		ana baba	ampio raiaco	outoutacou o
s1 wres	s1	Weight	plasma	t
	4.475e+004	-	-	0.000e+000
1.391e+000	4.461e+004	4.104e-007	4.678e+004	7.000e-003
-2.519e-001	4.389e+004	4.741e-007	4.352e+004	4.200e-002
2.117e-001	4.223e+004	4.964e-007	4.254e+004	1.250e-001
1.772e-001	3.989e+004	5.578e-007	4.013e+004	2.500e-001
-1.225e+000	3.770e+004	6.845e-007	3.622e+004	3.750e-001
-8.650e-002	3.566e+004	7.101e-007	3.556e+004	5.000e-001
-	3.200e+004	-	-	7.500e-001
-6.469e-001	2.880e+004	1.130e-006	2.819e+004	1.000e+000
-	2.405e+004	-	-	1.450e+000
-	2.166e+004	-	-	1.725e+000
-4.317e-002	1.960e+004	2.344e-006	1.957e+004	2.000e+000
-	1.680e+004	-	-	2.450e+000
-	1.537e+004	-	-	2.725e+000
5.867e-001	1.412e+004	4.329e-006	1.440e+004	3.000e+000
-	1.240e+004	-	-	3.450e+000
-	1.151e+004	-	-	3.725e+000
1.494e+000	1.072e+004	7.061e-006	1.128e+004	4.000e+000
-	9.603e+003	-	-	4.450e+000
-	9.016e+003	-	-	4.725e+000

5.000e+000 5.450e+000 6.000e+000 6.450e+000 6.725e+000 7.000e+000 7.450e+000 8.000e+000 8.450e+000 8.450e+000 8.725e+000 9.000e+000	8.081e+003 - - 6.999e+003 - - 5.653e+003 - - 5.139e+003 - - - - - - - - - - - - -	1.375e-005  1.833e-005  2.810e-005  3.401e-005  	8.487e+003 7.728e+003 7.319e+003 6.944e+003 6.395e+003 5.813e+003 5.396e+003 5.162e+003 4.943e+003 4.612e+003 4.424e+003 4.246e+003	-1.507e+000  2.355e-001  -8.504e-001  1.142e+000  	
9.000e+000 9.000e+000	_ 4.210e+003	_ 5.067e-005	4.246e+003 4.246e+003	-2.582e-001	

Statistics

Parameter/Variable Value	Std.Dev. Coef. of Var.	95% Confidence Interval	
k(0,1)         0.29227         1.461           k(1,2)         0.28311         7.511           k(2,1)         0.17452         1.826           vol         2323.77661         3.856	55e-002 5.00071e+000 83e-002 2.65335e+001 36e-002 1.04652e+001 619e+001 1.65945e+000	0.260100.324440.117770.448440.134320.214722238.902192408.65103	
sl : plasma	Objective So 1.336743e+001	caled Data Variance 1.113515e-001	
Total objective	1.336743e+001		
AIC BIC	7.935987e+000 8.053995e+000		
Number of Iterations Re	equired to Fit: 5		
Notes			
None			

The information parallels that following the Solve except now information on the Fit is available. This includes the weights and weighted residuals, and the information from the **Statistics** window. It also includes the number of iterations required to Fit the data.

c. Close the text file and return to **study\_0**.

This information can be cut from the text window and pasted into another application for you to prepare your report.

Quit the SAAM II Compartmental application. Do not save the changes to study\_0.