Aspen Tutorial #2: Convergence and Presentation of Results

Outline:

- Problem Description
- Checking Simulation Results
- Adding Stream Tables
- Adding Stream Conditions
- Printing from Aspen
- Viewing the Input Summary

Problem Description:

A mixture containing 50.0 wt% acetone and 50.0 wt% water is to be separated into two streams – one enriched in acetone and the other in water. The separation process consists of extraction of the acetone from the water into methyl isobutyl ketone (MIBK), which dissolves acetone but is nearly immiscible with water. The overall goal of this problem is to separate the feed stream into two streams which have greater than 90% purity of water and acetone respectively.

This week we will be learning about some of the features that Aspen has for presenting simulation results. We will also be covering the importance of checking for convergence and making sure that the solutions determined by Aspen are reasonable. We will be using our simulations from last week to cover these topics.

Checking Simulation Results:

One of the most important things to remember when using a computer simulation program, in any application, is that incorrect input data or programming can lead to solutions that are "correct" based on the program's specifications, but unrealistic with regards to real life applications (i.e. a distillation tower that can split crude oil into fuel gas, gasoline, and asphalt on only one tray). For this reason it is very important that the user complete at least some very basic checks and balances to make sure the simulation results are reasonable, based on their experience and the expected results.

At the end of Tutorial #1 we had completed a simulation of the first mixer in our acetone separation process. Reopen your simulation by using the "Open an Existing Simulation" option. Because this tutorial was focused on learning the basics of Aspen, we did not discuss checking your results. For this reason we will rerun our existing simulation.

To do this we must first reinitialize our simulation in order to delete the existing results. This can be done by going to Run/Reinitialize in the menu bar. After selecting OK for both of the windows that pop up when you select the reinitialize option, your simulation will be reset (Note: This feature is useful when modifying an existing simulation and we will use it a lot this quarter). Now that the simulation has been reset, run it again, but this time use the next button. By using the next button to run the simulation, the program will

show you information about its convergence in a status window that otherwise does not normally appear. If you run the simulation in another fashion, this status window can be opened by selecting the Run Control Panel button in the toolbar. This window and the Run Control Panel button can be seen in Figure 1.

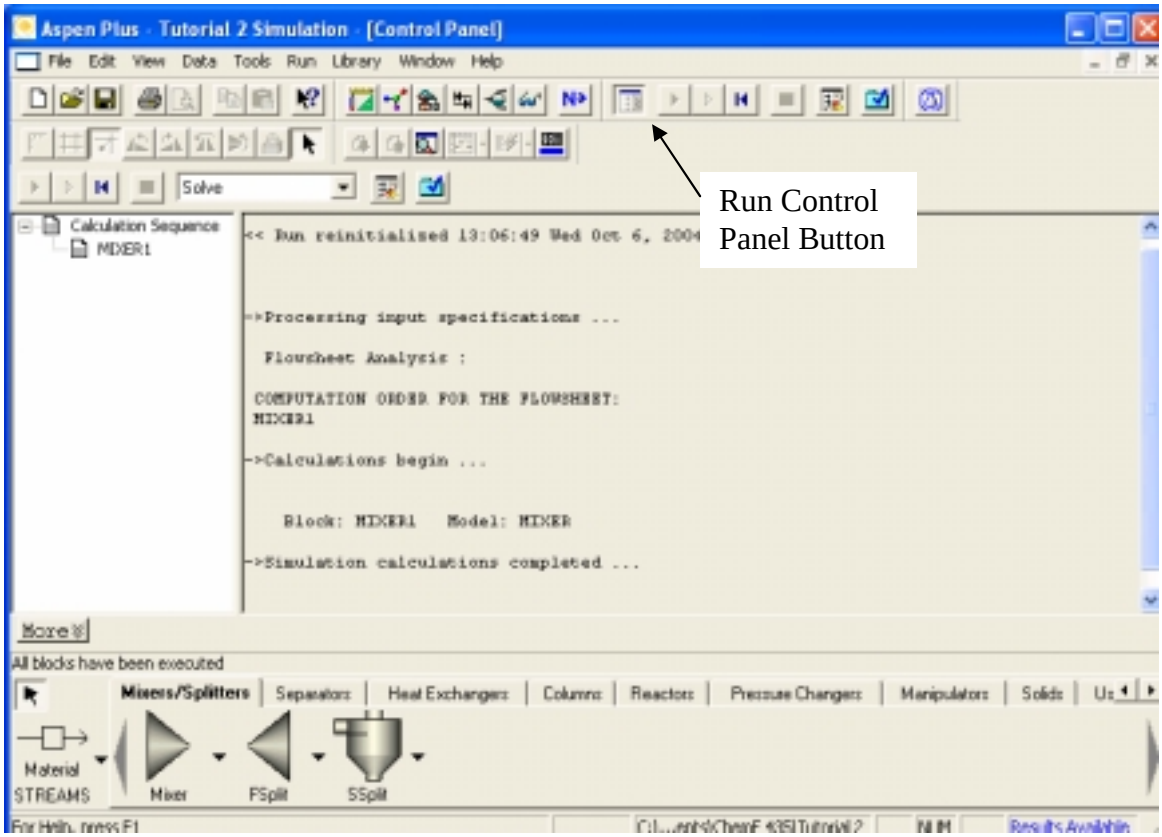


Figure 1: Convergence Status Window

Because our simulation is a very basic system you should not have convergence difficulties. However, as our simulation progresses over the quarter, we will be adding more complicated unit operations (equipment) which may require multiple iterations to solve. In this case you will want to examine this status window closely to make sure that the simulation did converge with reasonable tolerance. Some factors that lead to convergence difficulties are a poor choice for the Base Method (thermodynamics) and the addition of recycle streams. This status window will also list any warnings or errors that may arise based on your input choices.

While our simulation converged normally, it does not necessarily mean that the solution is reasonable. We will now proceed on to another basic check that should be done when completing simulations. Close the status window by selecting the Run Control Panel button. When this window is closed open up the Data Browser window.

Click on the Results Summary Tab and open up the Streams option. When you do this you will be presented with a stream material summary table. While we expect Aspen to be correct, it is advisable to run a few simple checks on the data presented in this table.

As mentioned above, Aspen can give "correct" but unreasonable results due to convergence or the selected thermodynamics, so it is highly recommended that you verify the results presented in this table. Some checks to perform include a quick material balance, a quick heat balance, and a comparison to experimental or operating data if it is available. Further along in your careers, you will be able to use your experience to notice much more quickly if the results do not appear to be reasonable. However, even then you should look at every number that is presented in the results. If your results appear to be acceptable you can move on to adding the simulation results to the process flowsheet for ease of presenting.

Adding Stream Tables:

Adding stream tables to the process flowsheet is a simple process, but we will first go over some options for formatting and modifying your stream tables. On the current screen you will see two of the options for varying the stream table: Display and Format. Under the Display drop down menu there are two options, all streams or streams. The streams option allows the user to choose which streams they would like presented, one by one. Under the Format drop down menu there are a number of types of stream tables. Each of the options presents the data in a slightly different fashion, depending on the intended application. We will use the CHEM_E option this quarter. To add a stream table, simply click on the Stream Table button and a stream table will be added to your process flowsheet. These features are highlighted in Figure 2.

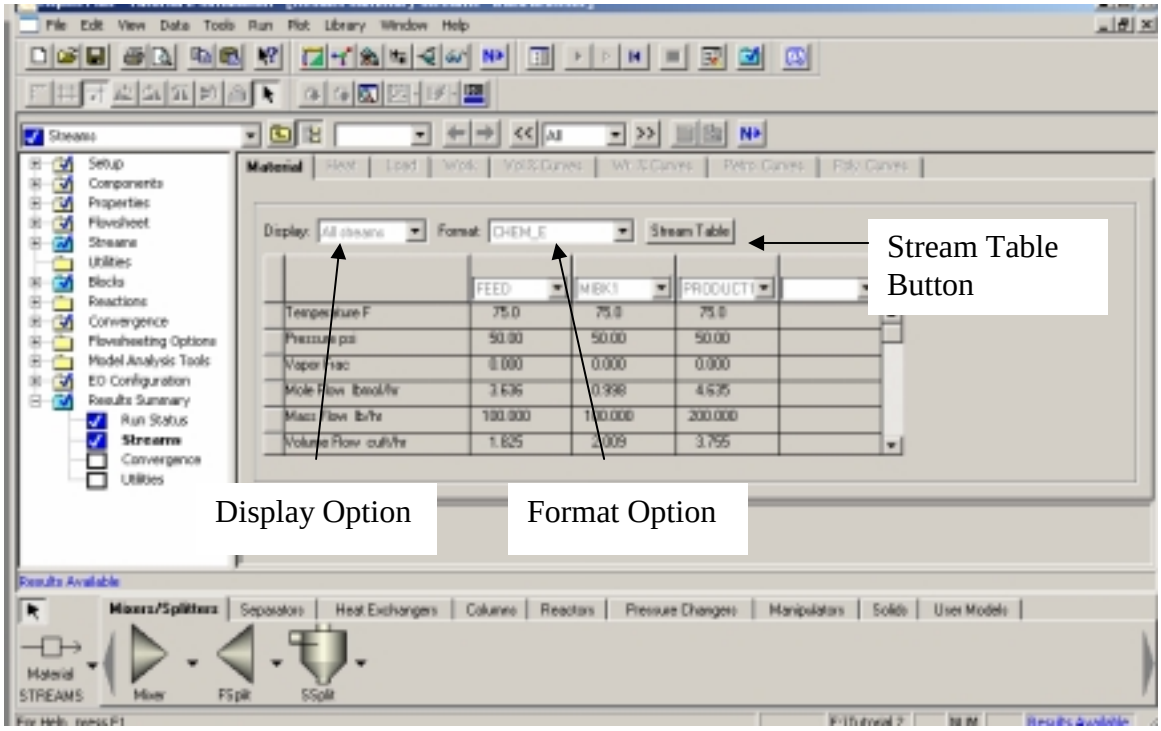
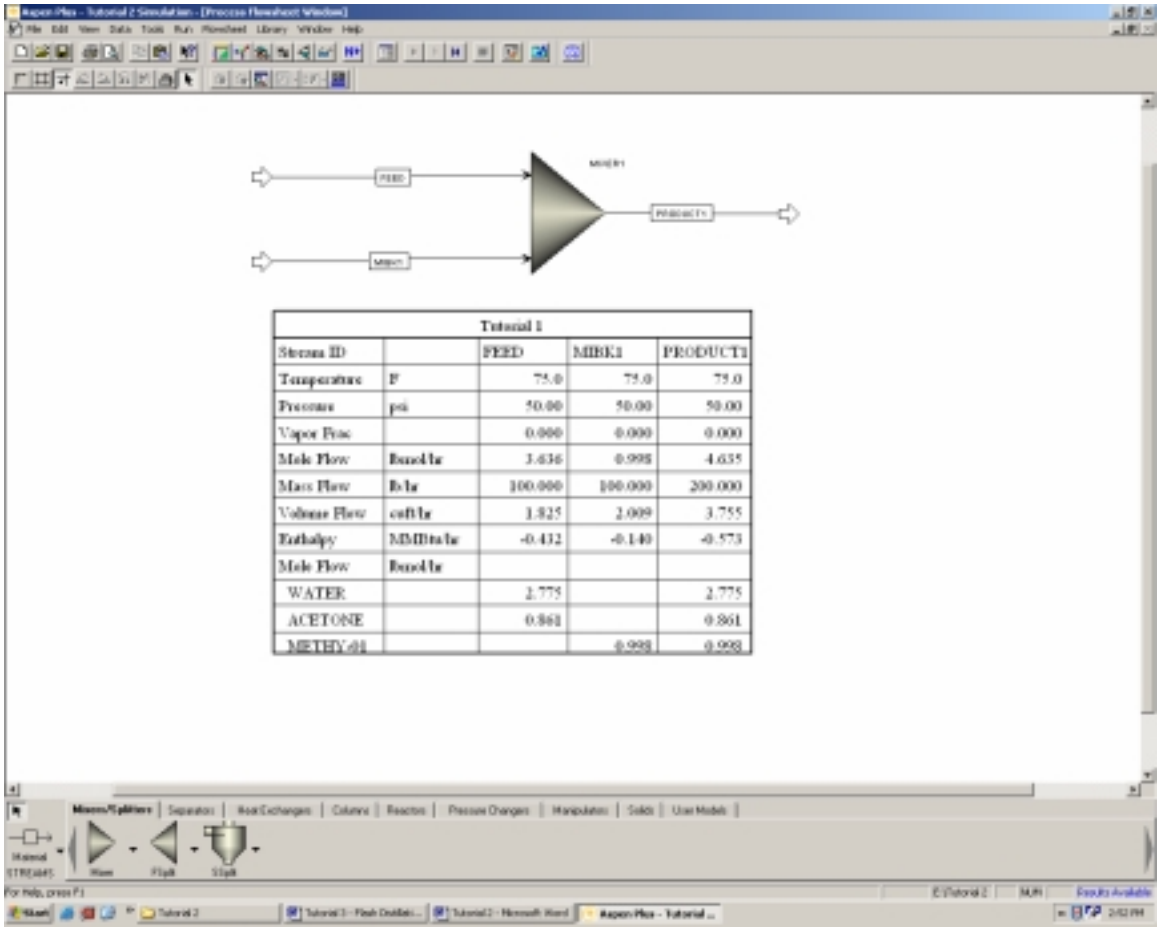


Figure 2: Stream Table Results

After you have added a stream table your process flowsheet should look similar to that seen in Figure 3.



Tutorial 1				
Stream ID		FEED	MIBK1	PRODUCT1
Temperature	F	75.0	75.0	75.0
Pressure	psi	50.00	50.00	50.00
Vapor Frac		0.000	0.000	0.000
Mole Flow	lbmol/hr	3.636	0.998	4.635
Mass Flow	lb/hr	100.000	100.000	200.000
Volume Flow	cuft/hr	1.825	2.009	3.755
Enthalpy	MMBtu/hr	-0.432	-0.140	-0.573
Mole Flow	lbmol/hr			
WATER		2.775		2.775
ACETONE		0.861		0.861
METHY-01			0.998	0.998

Figure 3: Process Flowsheet with Stream Table

There is one other location where the user can modify the appearance and content of stream tables. In the Data Browser window, under the Setup tab there is an option entitled Report Options. In this option there is a tab labeled Stream which is shown in Figure 4. You will notice that the user can add to or reduce from the number of items to be included in the stream report (flow basis, fraction basis, etc.). The user can also change the sized of the stream format from standard to wide. However, if you change any of these features after your simulation has been run and converged, they will not appear in your stream table until you have rerun the simulation. At this point make sure that your stream table is set up to report the mole flow basis and the mass fraction basis, and rerun your simulation. Your process flowsheet should now look like that seen in Figure 5. You will notice the stream table that you have added to the process flowsheet should automatically update with the new stream table conditions that you have input. However, if it does not, simply click on the stream table and then click on the process flowsheet window and the table will update.

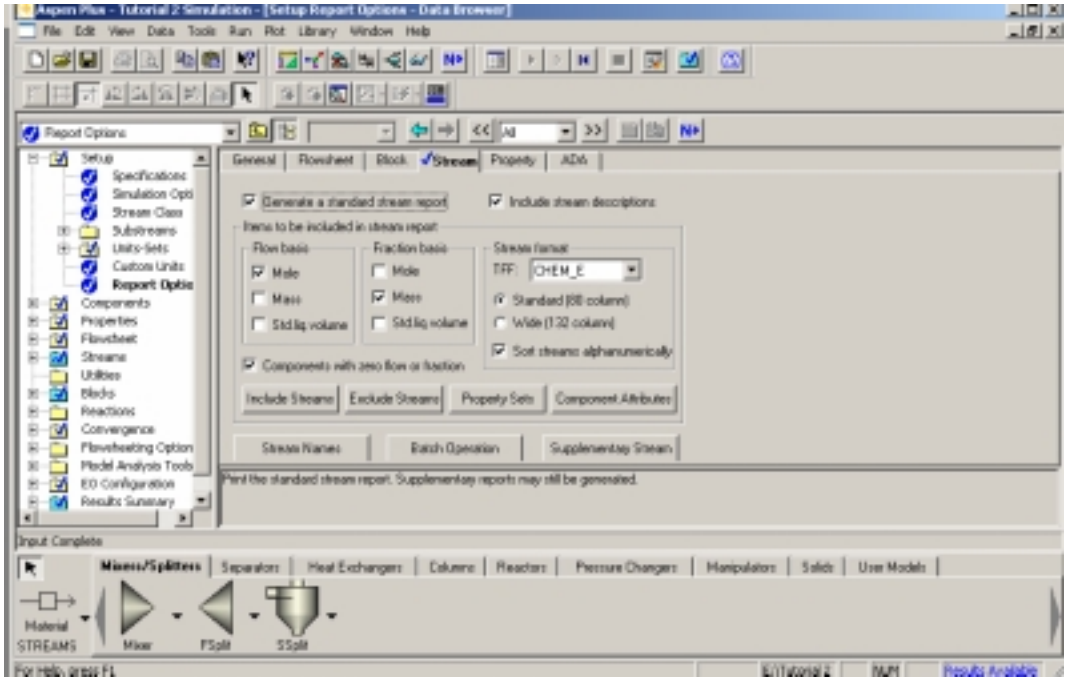
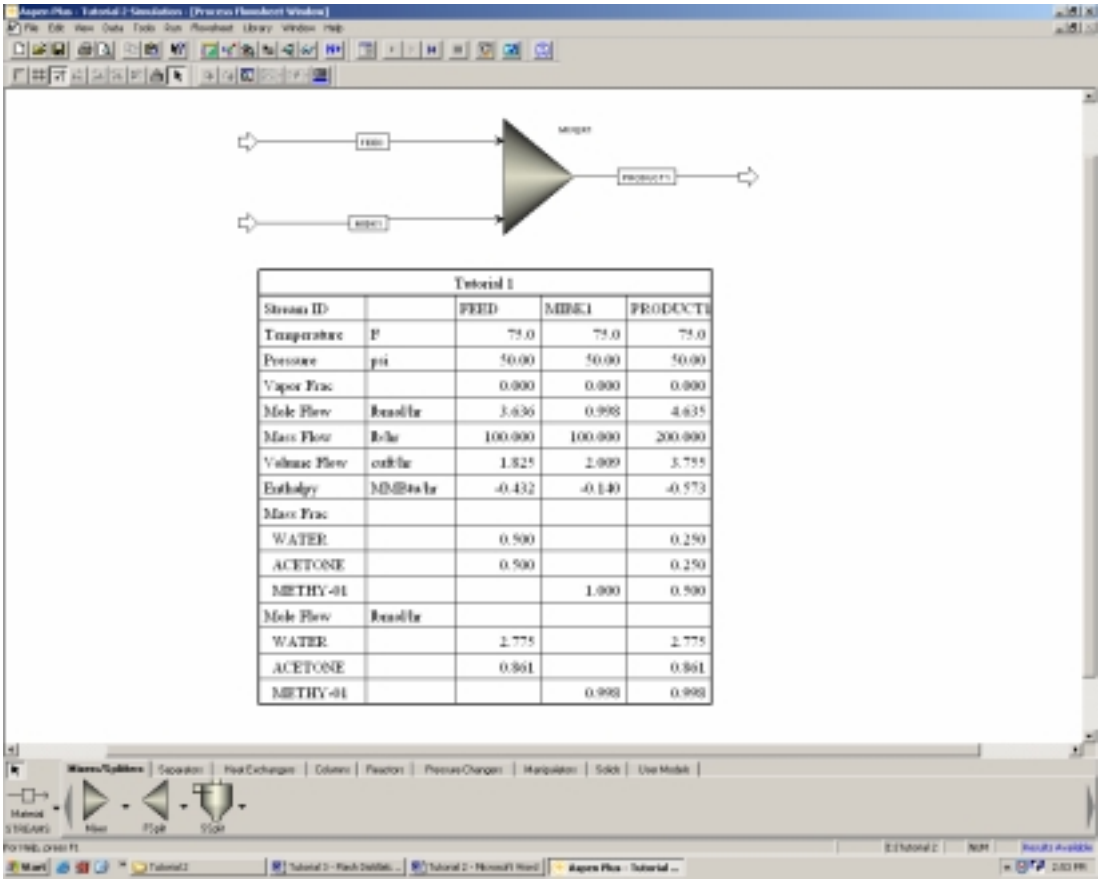


Figure 4: Stream Options



Tutorial 1

Stream ID		FEED	MIX1	PRODUCT1
Temperature	F	75.0	75.0	75.0
Pressure	psi	50.00	50.00	50.00
Vapor Frac		0.000	0.000	0.000
Mole Flow	lbmol/hr	3.636	0.998	4.635
Mass Flow	lb/hr	100.000	100.000	200.000
Volume Flow	cuft/hr	1.825	2.009	3.755
Enthalpy	MMBtu/hr	-0.432	-0.140	-0.573
Mass Frac				
WATER		0.500		0.250
ACETONE		0.500		0.250
METHY-01			1.000	0.500
Mole Flow	lbmol/hr			
WATER		2.775		2.775
ACETONE		0.861		0.861
METHY-01			0.998	0.998

Figure 5: Updated Stream Table

Adding Stream Conditions:

In a large simulation, it is often useful to add stream conditions directly to the streams themselves so the user doesn't have to search through a large stream table for values. While this is not the case in our simulation we will now add the temperature and pressure to each of the streams to learn how to do this.

This can be done in the Options window under Tools in the menu bar shown in Figure 6. When you have opened the Options window, click on the Results View Tab. Select the Temperature and Pressure options and hit OK. You will notice those two properties will now be shown on your process flow worksheet as shown in Figure 7. The format of these variables can be changed in the Options window by changing the symbology in the Format box. The only value you will likely change is the number in the box – this represents the number of decimal places in the displayed values. We will not change this now.

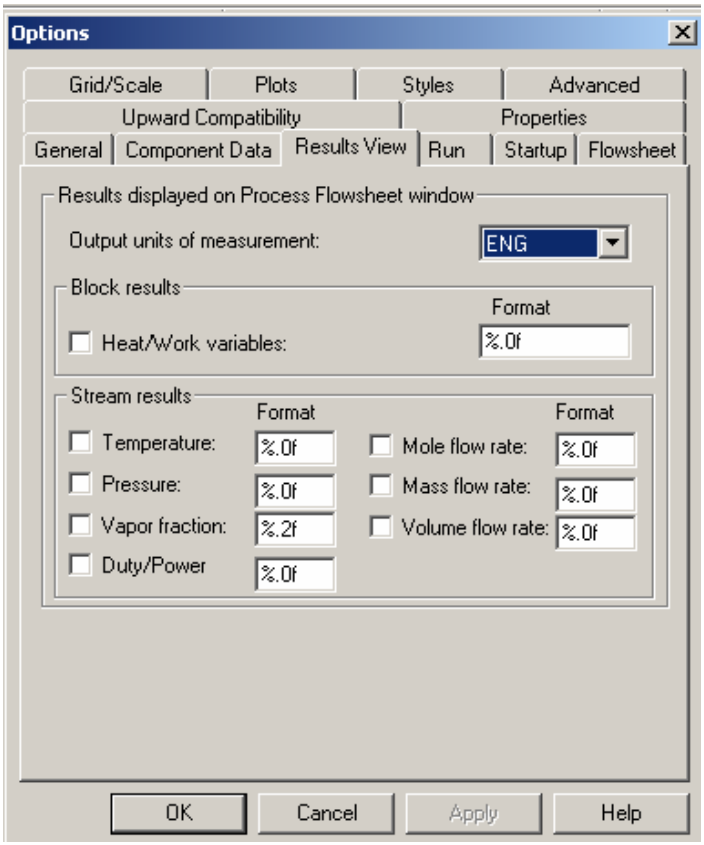
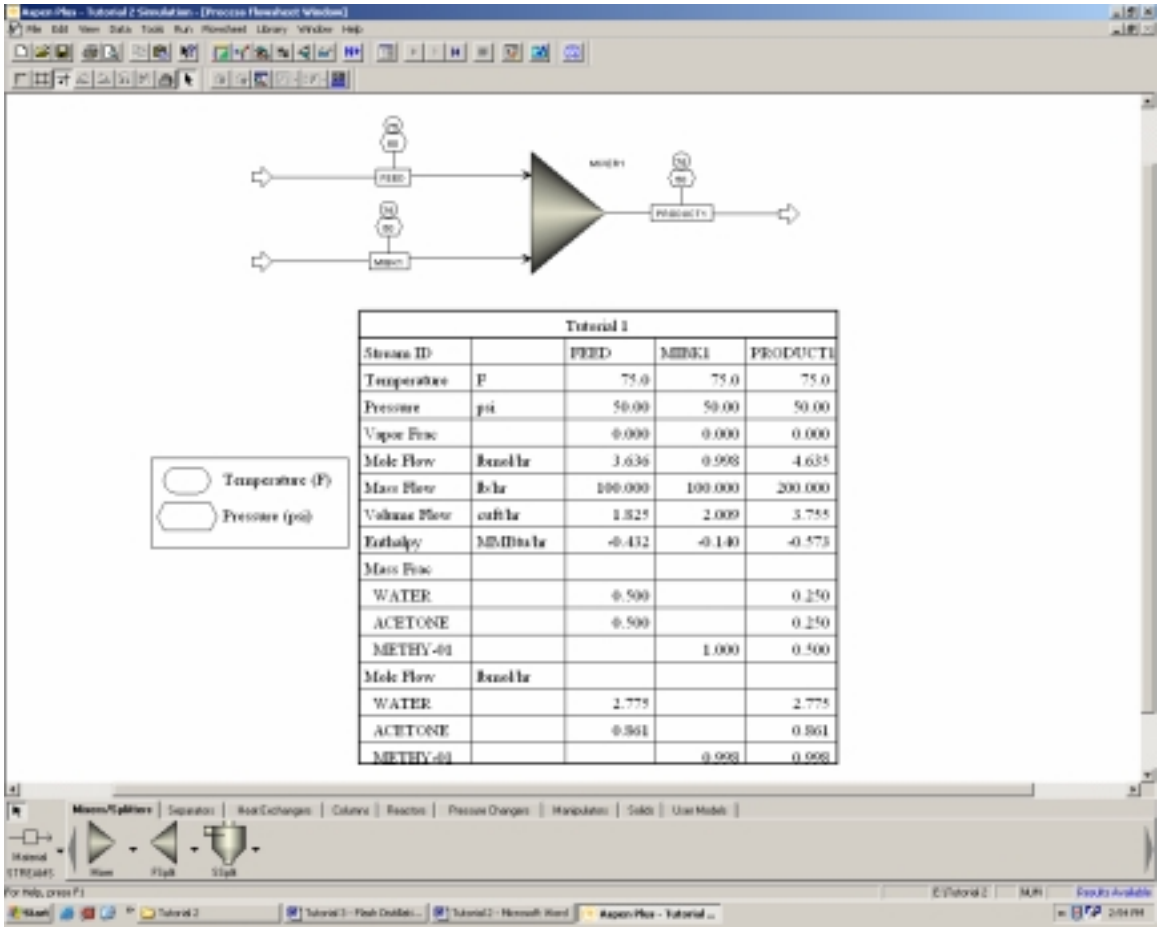


Figure 6: Options Window



Tutorial 1				
Stream ID		FEED	MIBK1	PRODUCT1
Temperature	F	75.0	75.0	75.0
Pressure	psi	50.00	50.00	50.00
Vapor Frac		0.000	0.000	0.000
Mole Flow	lbmol/hr	3.636	0.998	4.635
Mass Flow	lb/hr	100.000	100.000	200.000
Volume Flow	cuft/hr	1.825	2.009	3.755
Enthalpy	MMBtu/hr	-0.432	-0.140	-0.573
Mass Frac				
WATER		0.500		0.250
ACETONE		0.500		0.250
METHY-01			1.000	0.500
Mole Flow	lbmol/hr			
WATER		2.775		2.775
ACETONE		0.861		0.861
METHY-01			0.998	0.998

Figure 7: Updated Process Flowsheet

Printing from Aspen:

Printing a process flowsheet can be completed quite easily from the print button on the toolbar. However, the user may want to select only a portion of a process flowsheet to print. To do this, either right click on the flowsheet window and select Page Break Preview, or go to View/Page Break Preview in the menu bar. Doing so will place a grey box around your entire process diagram in the flowsheet window as shown in Figure 8. This box represents the area that will be printed, similar to the print preview option in other programs. This box can be moved around on the screen and/or reduced/enlarged to fit the user's need. When the box is positioned to the users need, the flowsheet can be printed as mentioned above.

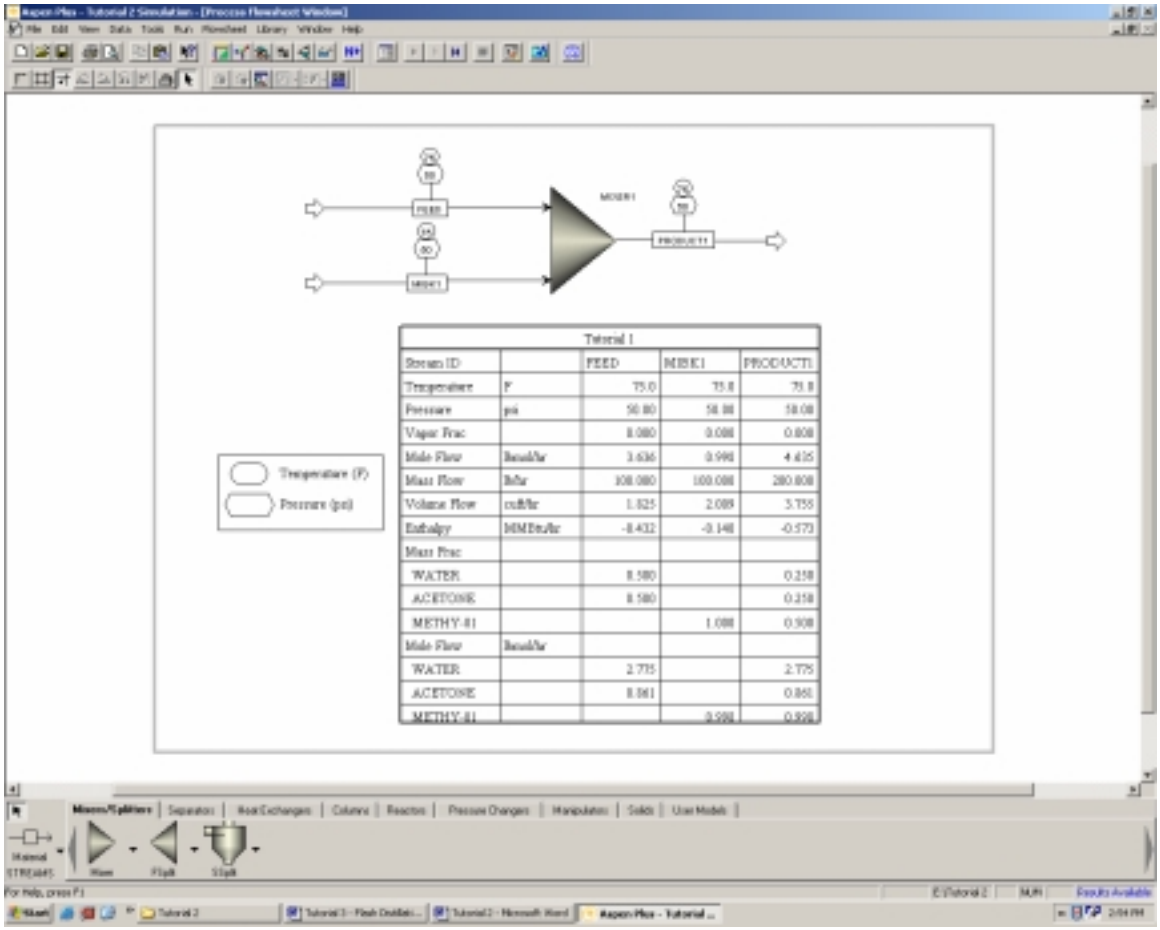


Figure 8: Page Break Preview

Viewing the Input Summary:

Another way for an Aspen user to present their results is through the program's Input Summary. This is a useful way to check your input data for errors (or for a supervisor to check a junior engineer's work quickly to look for bad assumptions etc.). The input summary is easily produced by going to View/Input Summary in the menu bar. The summary will be opened up in Notepad and it can be saved or printed directly from here.

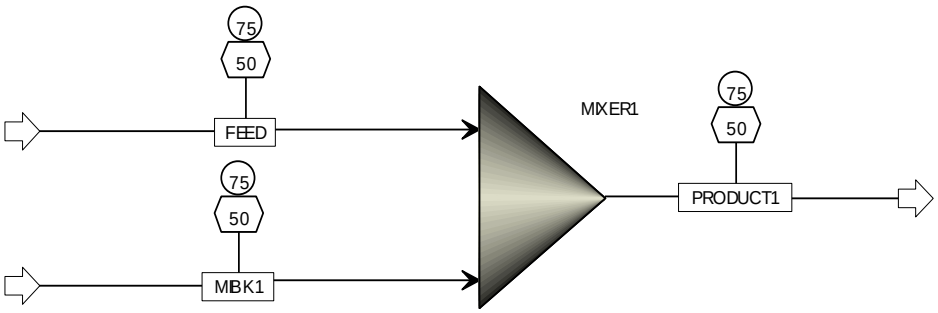
Next week: Flash Distillation

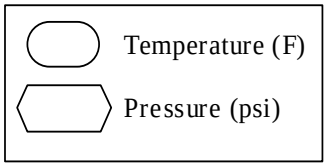
Tutorial #2 Homework and Solution

Question:

Turn in a copy of both the completed process flowsheet and the Input Summary that are created while working through Aspen Tutorial #2.

Solution:





Tutorial 1				
Stream ID		FEED	MIBK1	PRODUCT1
Temperature	F	75.0	75.0	75.0
Pressure	psi	50.00	50.00	50.00
Vapor Frac		0.000	0.000	0.000
Mole Flow	lbmol/hr	3.636	0.998	4.635
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Mass Frac				
WATER		0.500		0.250
ACETONE		0.500		0.250
METHY-01			1.000	0.500
Mole Flow	lbmol/hr			
WATER		2.775		2.775
ACETONE		0.861		0.861
METHY-01			0.998	0.998

```
;
;Input Summary created by Aspen Plus Rel. 12.1 at 14:57:13 Wed Oct 13,
2004
;Directory E:\Tutorial 2  Filename
C:\DOCUME~1\BERNAR~1\LOCALS~1\Temp\~ap58f.tmp
;

TITLE 'Tutorial 1'

IN-UNITS ENG

DEF-STREAMS CONVEN ALL

DESCRIPTION "
    General Simulation with English Units :
    F, psi, lb/hr, lbmol/hr, Btu/hr, cuft/hr.

    Property Method: None

    Flow basis for input: Mole

    Stream report composition: Mole flow
    "

DATABANKS PURE12  / AQUEOUS  / SOLIDS  / INORGANIC  /  &
        NOASPENPCD

PROP-SOURCES PURE12  / AQUEOUS  / SOLIDS  / INORGANIC

COMPONENTS
    WATER H2O /
    ACETONE C3H6O-1 /
    METHY-01 C6H12O-2

FLOWSHEET
    BLOCK MIXER1 IN=FEED MIBK1 OUT=PRODUCT1

PROPERTIES IDEAL

STREAM FEED
    SUBSTREAM MIXED TEMP=75. PRES=50. MASS-FLOW=100.
    MASS-FRAC WATER 0.5 / ACETONE 0.5 / METHY-01 0.

STREAM MIBK1
    SUBSTREAM MIXED TEMP=75. PRES=50. MASS-FLOW=100.
    MOLE-FRAC METHY-01 1.

BLOCK MIXER1 MIXER
    PARAM NPHASE=1 PHASE=L
    BLOCK-OPTION FREE-WATER=NO

EO-CONV-OPTI

STREAM-REPOR NARROW MOLEFLOW MASSFRAC
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