Aspen Tutorial #1: Aspen Basics

Outline:

- Introduction to Aspen
- Problem Description
- Beginning a Simulation
- Navigating the Aspen Window
- Creating a Process Flowsheet
- Data Input
- Running the Simulation

Introduction:

In industry complicated problems are often not solved by hand for two reasons: human error and time constraints. There are many different simulation programs used in industry depending on the field, application, and desired simulation products (entire process unit, one piece of equipment, etc.). When used to its full capabilities, Aspen can be a very powerful tool for a Chemical Engineer in a variety of fields including oil and gas production, refining, chemical processing, environmental studies, and power generation to name a few.

Over the course of these tutorials, you will be introduced to some of the basic features of Aspen as we build a simulation of an acetone/water extraction-distillation process. This problem is based very loosely on Example Problem 4.4-2 in Elementary Principles of Chemical Process by Felder and Rousseau. Because we will build on our existing simulation with each tutorial, it is highly recommended that you save your work every week so you do not have to start from scratch each time. The homework problems will emphasize one particular feature of Aspen that is covered in the tutorial for that week.

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 begin by learning the basics of running Aspen and building a process flowsheet. This will be one of the longest tutorials of the quarter as it introduces you to a number of features that must be understood to complete even a basic simulation. Our goal at the end of this tutorial is to understand some of the features of Aspen while creating a simulation of the mixture of a feed stream of 100 lbs/hr of the 50/50 acetone-water mix with a solvent stream of 100 lbs/hr of MIBK.

Beginning a Simulation:

1. Start the Aspen program. It can be found in the start menu under:
   Start/Programs/ChemE/Aspen Plus User Interface
2. Choose what type of simulation you would like to use. Later on in the quarter you will want to open up an existing simulation, but now we will use the template option.

   The window that appears can be seen in Figure 1. I mention it to again highlight the variety of problems that Aspen can solve as seen by the number of available templates.

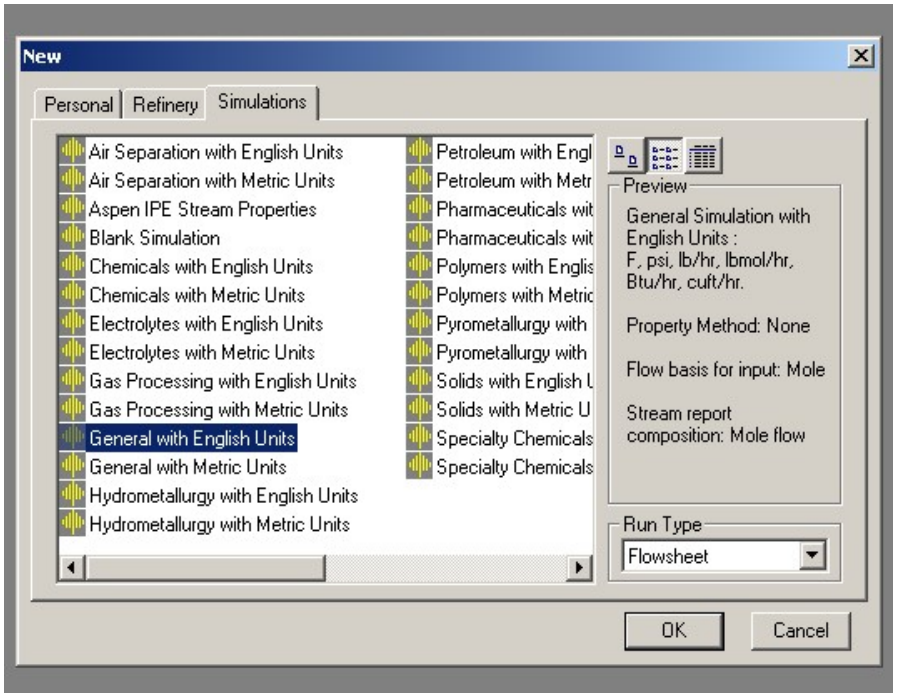


Figure 1: Available Simulation Templates

   We will use the General with English Units option.

3. When the Connect to Engine window appears, use the default Server Type (Local PC).

Navigating the Aspen Window:

Figure 2, on the next page shows the Aspen process flowsheet window. Some of the features are highlighted in the Figure and the most general of these will be discussed in the sections that follow.

Some things worth mentioning:

- Your simulation efforts will be greatly aided by becoming familiar with the toolbar features. This will eliminate the need to search through the menu bar for the various features.
- Hitting the arrow on the side of either a piece of equipment or the stream will present a number of options for that particular item.
- The status bar will tell the user what each piece of equipment will do. This is useful when selecting pieces of equipment like columns or reactors for more complicated simulation work.
- The simulation status in the bottom right hand corner will notify the user when all of the required data has been input and the simulation can be run.

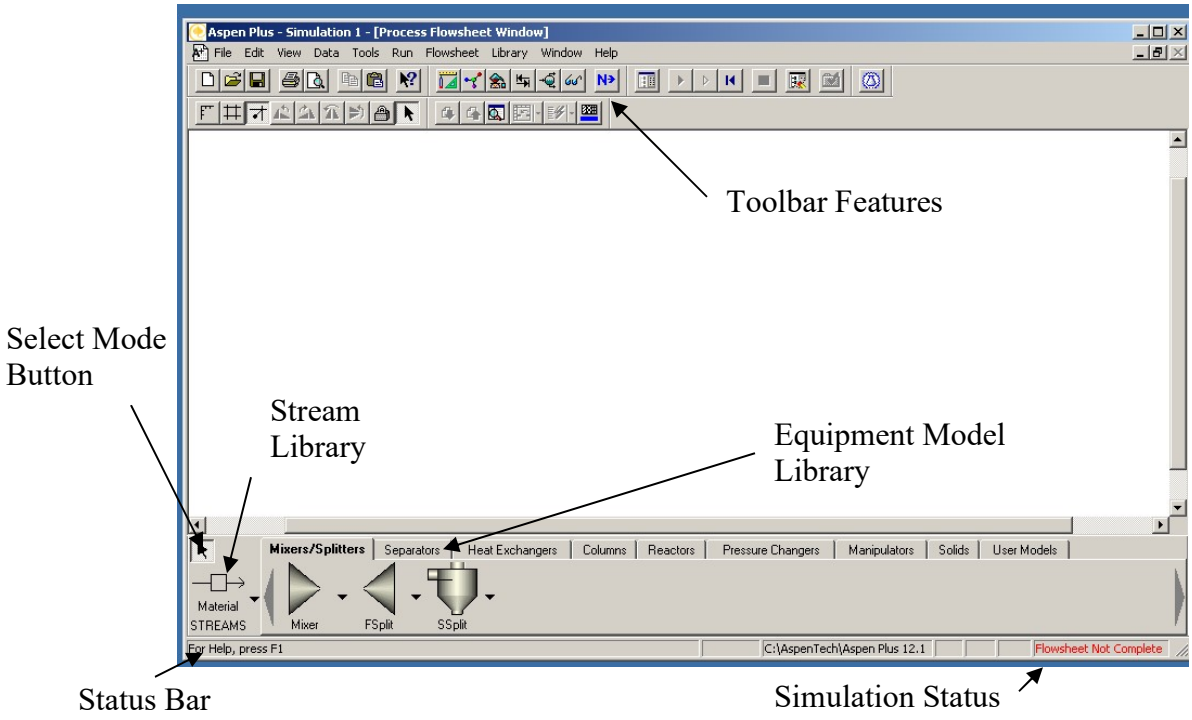


Figure 2: Process Flowsheet Window

Creating a Process Flowsheet:

To place a unit operation (or piece of equipment) into the flowsheet window, select it from the Equipment Model Library and then click on the flowsheet window where you would like the piece of equipment to appear. Do this for each piece of equipment that you would like to add to your simulation. For this week's simulation you will only need to add one Stream Mixer (found in the Mixers/Splitters Tab). You may want to go through the rest of the Equipment Model Library to see what other types of equipment are available in this program.

It should be pointed out that after adding your desired unit operations you must click on the Select Mode Button to reposition or resize the icon. If you do not select this button, you will continue to add equipment to the process flowsheet. To delete extraneous equipment, simply highlight that object and hit the delete key on the keyboard.

To add Material Streams to your simulation select the appropriate stream from the Stream Library (other options include heat and work, but we will not be using those at this time). It should be pointed out that Aspen has a feature that will indicate to you where streams are required. When you select the material stream option, a number of arrows will appear on each of the unit operations. Red arrows indicate a required stream and blue arrows indicate an optional stream. This is shown in Figure 3 below.

Streams can be added by clicking on the process flowsheet where you would like the stream to begin and clicking again where you would like the stream to end. To connect to a piece of equipment you must have the desired stream type selected and then begin or end on one of the arrows shown on the piece of equipment (depending on if your stream is a feed to or product from the equipment). In a similar fashion to the equipment, each click will add a new stream to the process flowsheet until you click on the Select Mode Button.

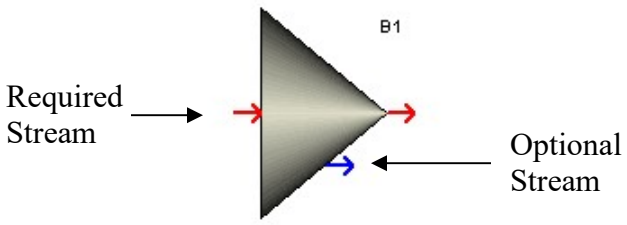


Figure 3: Required Stream Locations

For this tutorial, you will need to add two streams feeding into the mixer, and one product stream leaving the mixer.

Some features of Aspen that should be mentioned at this point are the ability to rotate, resize, and rename both the streams and the unit operations. To do this, simply select the object that you would like to manipulate and right click on it. This will present you with a number of options for changing each object. I would recommend renaming both the material streams and the mixer to names that will better distinguish them (rather than the default numbers and letters).

At this point your process flowsheet should be complete and it should somewhat resemble the one shown in Figure 4. Notice the simulation status has been changed from "Flowsheet not Complete" to "Required Input Incomplete".

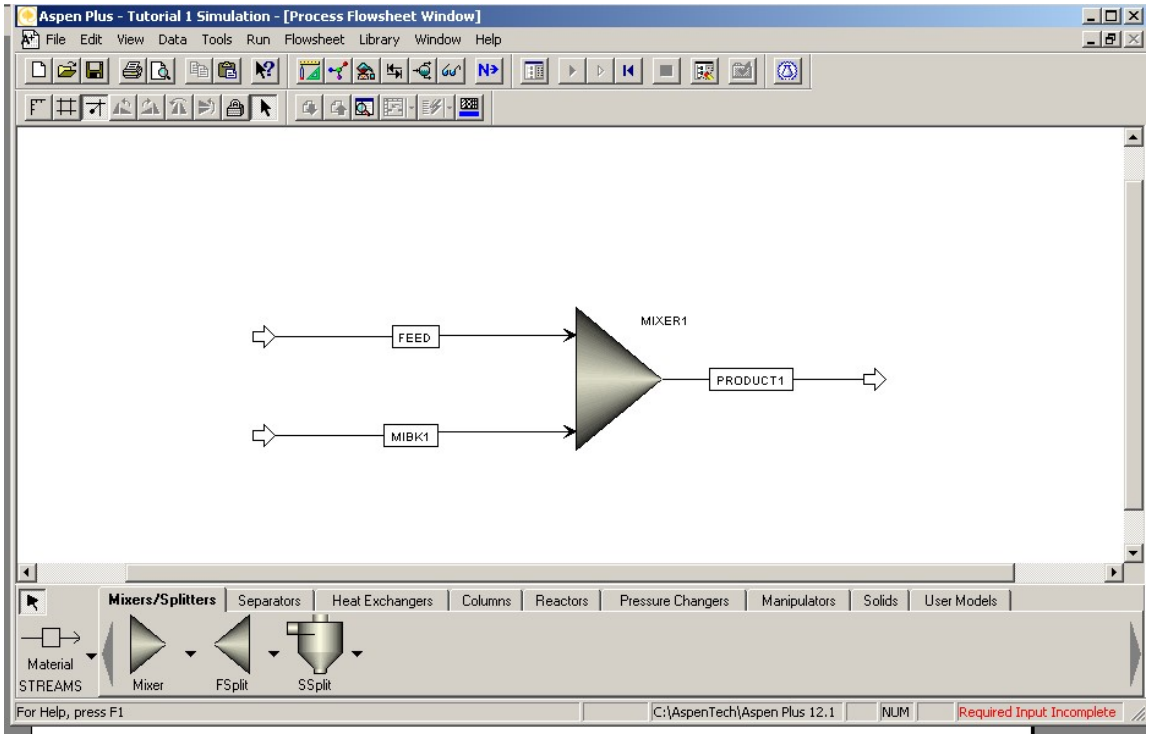


Figure 4: Completed Mixer Flowsheet

Data Input:

All of the data input for Aspen is entered in the Data Browser window. This window can be opened by clicking on the eyeglass icon or by going to Data/Data Browser in the Menu Bar. Aspen has two features in the Data Browser window that can both help and hurt the user. The first of these can be seen on the right hand side. Aspen highlights the areas where the input has been complete and has not been completed with the use of either a blue check mark or a half filled red circle, as seen in Figure 5. However, you can not always assume that all of the required input has been entered, especially if you are simulating a more complex problem. This feature will only track the minimal data input required to run a simulation and may cause problems in getting simulations to converge successfully. I recommend going through each icon on the left hand side one by one to make sure that you input all of the desired data for your particular application.

Aspen also has a tool in the toolbar that will automatically take the user through the required data input in a stepwise fashion. The button that does this is the blue N with the arrow (Next), also seen in Figure 5. Again, this feature steps through only the minimal data input and I would recommend avoiding the use of it until you are more experienced with Aspen.

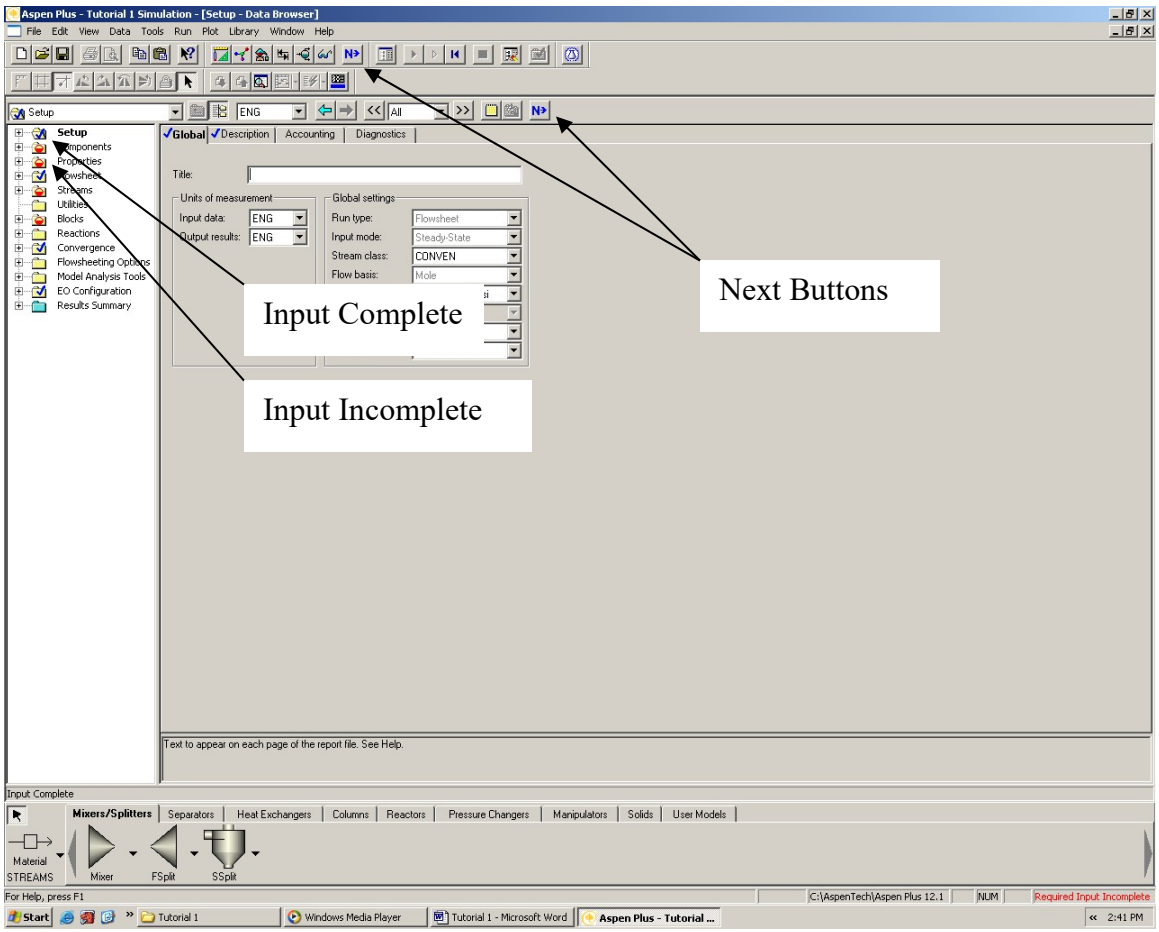


Figure 5: Data Browser Window

Under the Setup tab, in the Specifications folder you can input features such as a simulation title and a description of the project that you are working on. These are useful features for tracking your work and for tracking changes that you make to your work over time. Other features that are worth mentioning are the Units-Sets option and the Report Options. In the Units-Sets tab a user can input a new base set of units based on what they would like for their specific application. For now we will stick with the default base set. Under the Report Options the user can change how and what information is provided after a simulation is completed and converged. We will discuss this more thoroughly in next week's tutorial.

Under the Components tab the user will input what components will be used in this simulation. Aspen has a huge database of commonly used (and some not so commonly used) components and their physical properties. It also has an option where a user can define components that are not included in the database. Under the Specifications option we will input our components in the Selection tab. In the box marked component name, enter each of the components one at a time and hit the enter key. When you enter Methyl Isobutyl Ketone the find wizard will open up. Select MIBK from the list of possible matches, hit the add button, and then close the find window. You must also input a Component ID for all of the components (although a default one will appear for MIBK).

If you do not, the program will not recognize that component later on. When you have entered all three components your screen should look similar to that in Figure 6.

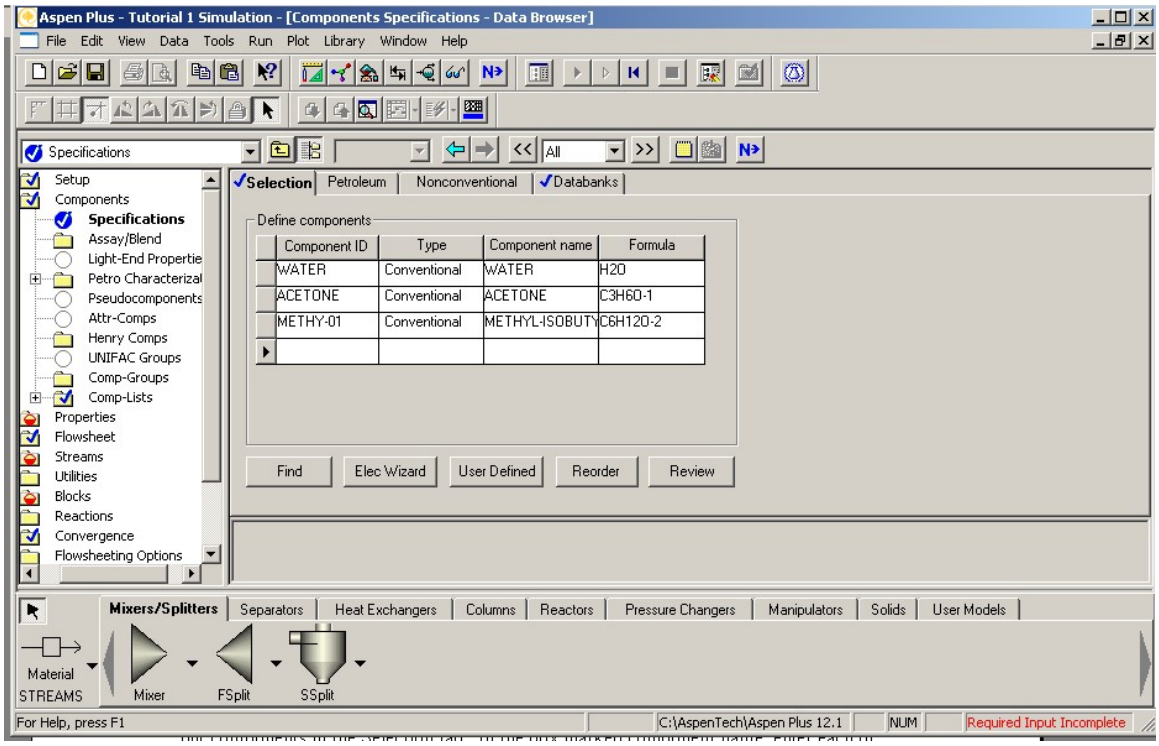


Figure 6: Component Selection

This is the only option where we will need to input data under the Components tab. It should be noted that there are a number of options for entering pseudo components or refining crude assays, etc. which is a commonly used feature in some industrial applications.

The user input under the Property tab is probably the most critical input required to run a successful simulation. This key input is the Base Method found under the Specifications option. The Base Method is the thermodynamic basis for all of the simulation calculations and this will be discussed in much greater detail in a later tutorial. For now select the Ideal method. In future applications, you may wish to use a Process type that is specific to your particular project. However, for now we will stick with the default All and this will complete our inputs under the Properties tab. The completed Property tab screen is shown in Figure 7.

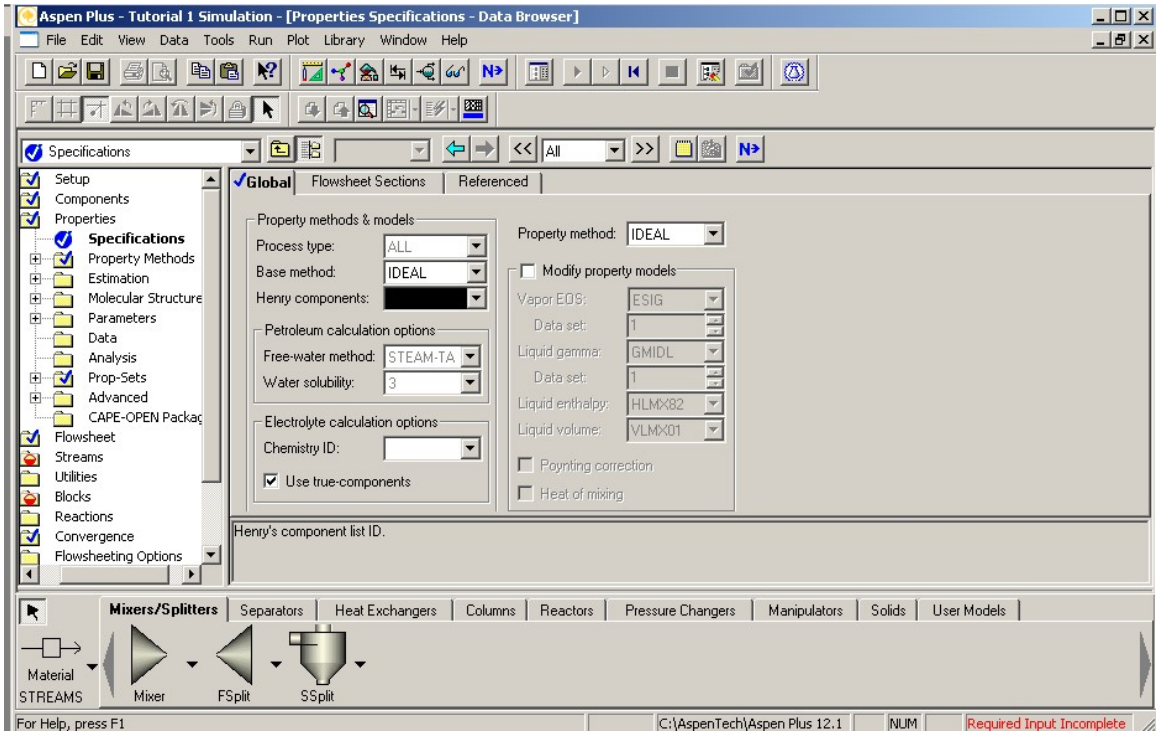


Figure 7: Completed Properties Screen

Under the Streams tab, we will enter in all of the specifications for each of the feed streams one at a time. Remember one feed stream is 100 lbs/hr of a 50/50 wt% mixture of Acetone and Water and the other stream is 100 lbs/hr of pure MIBK. For this simulation we will use a temperature of 75° F and a pressure of 50 psi. Take notice of the many ways you can input the stream data (i.e. temperature/pressure/vapor fraction, mole/mass basis, and stream compositions based on percent flow/mass flow/mole flow etc.). Input the appropriate data for both your feed and solvent streams (mine are named Feed and MIBK1). You will either need to switch the basis for the streams or do some hand calculations to convert the problem's mass flow to the default mole flow (I suggest switching the basis). When complete, the window should look like the one seen in Figure 8.

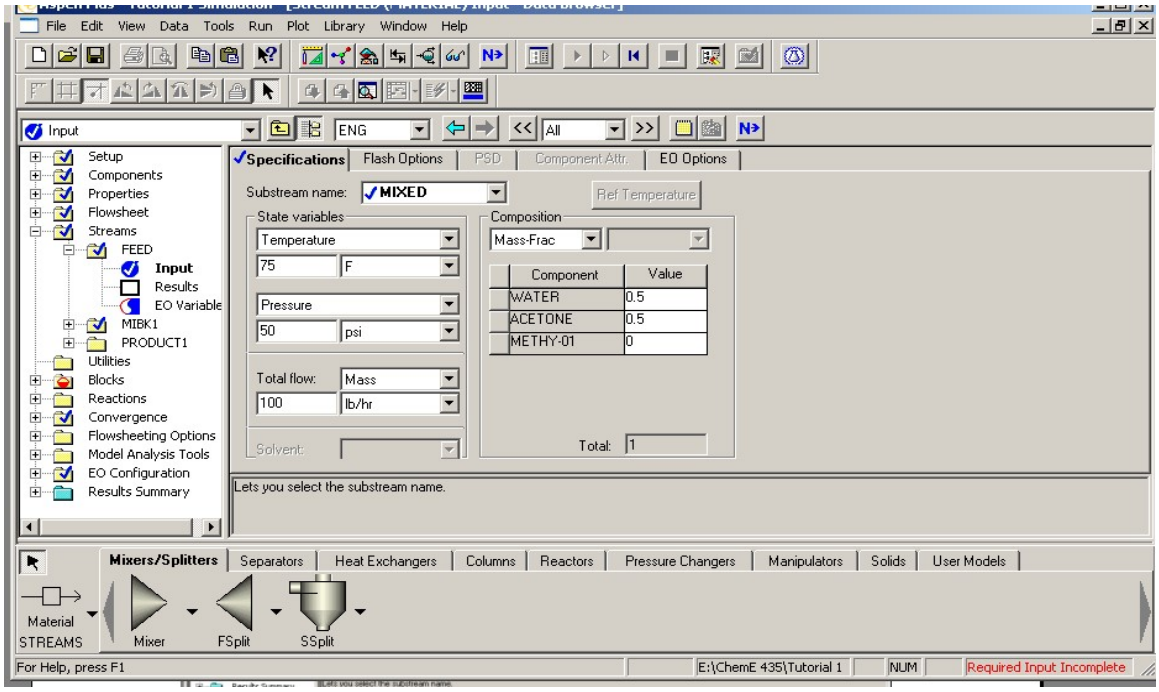


Figure 8: Completed Feed Stream Input

The final area that requires input is the Blocks tab. Open up this feature and the tab corresponding to the mixer. Under this unit operation we have the option of forcing the feed streams to mix at a desired pressure or with valid phases. In our mixer we are not changing the temperature or pressure so we will specify that liquids are the only valid phases because both of the feed streams are liquid at these conditions. After this is input you will notice that the Simulation Status changes to "Required Input Complete".

There are a number of other features in the Data Browser that we will work with over the course of the quarter, but for now our input is complete and you are ready to run the simulation.

Running the Simulation:

There are a few ways to run the simulation. The user could select either the Next button in the toolbar which will tell you that all of the required inputs are complete and ask if you would like to run the simulation. The user can also run the simulation by selecting the run button in the toolbar (this is the button with a block arrow pointing to the right). Finally, the user can go to run on the menu bar and select run.

After the simulation is run and converged, you will notice that the Results Summary Tab on the Data Browser Window has a blue check mark. Clicking on that tab will open up the Run Status. If your simulation has converged it should state "Calculations were completed normally". If you have received this message you have successfully completed Tutorial #1.

Next week: Convergence and Presentation of Results

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.

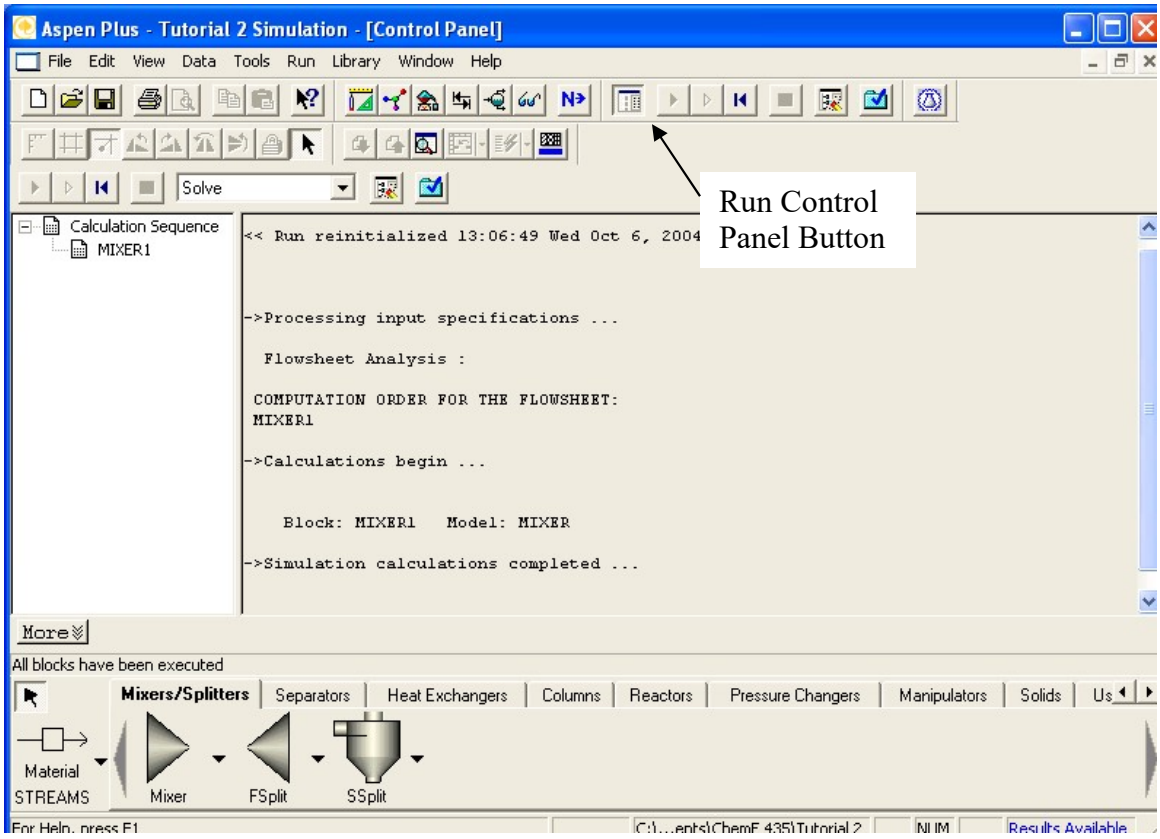


Figure 1: Convergence Status Window

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.

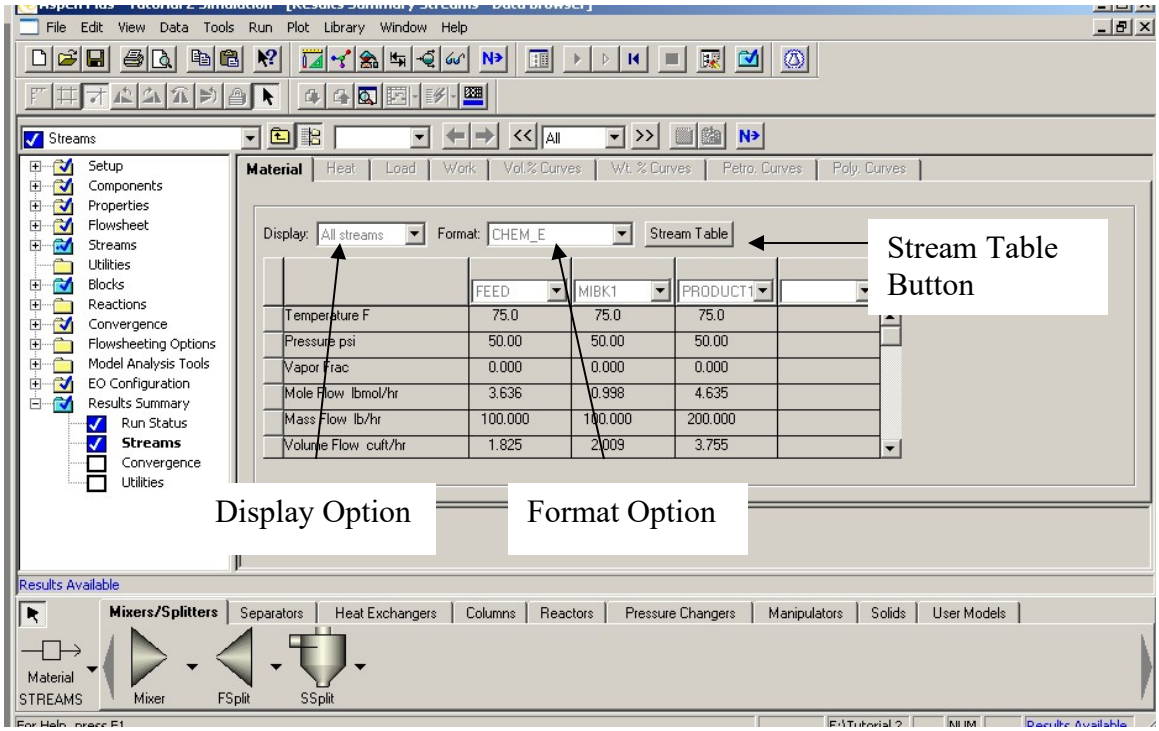
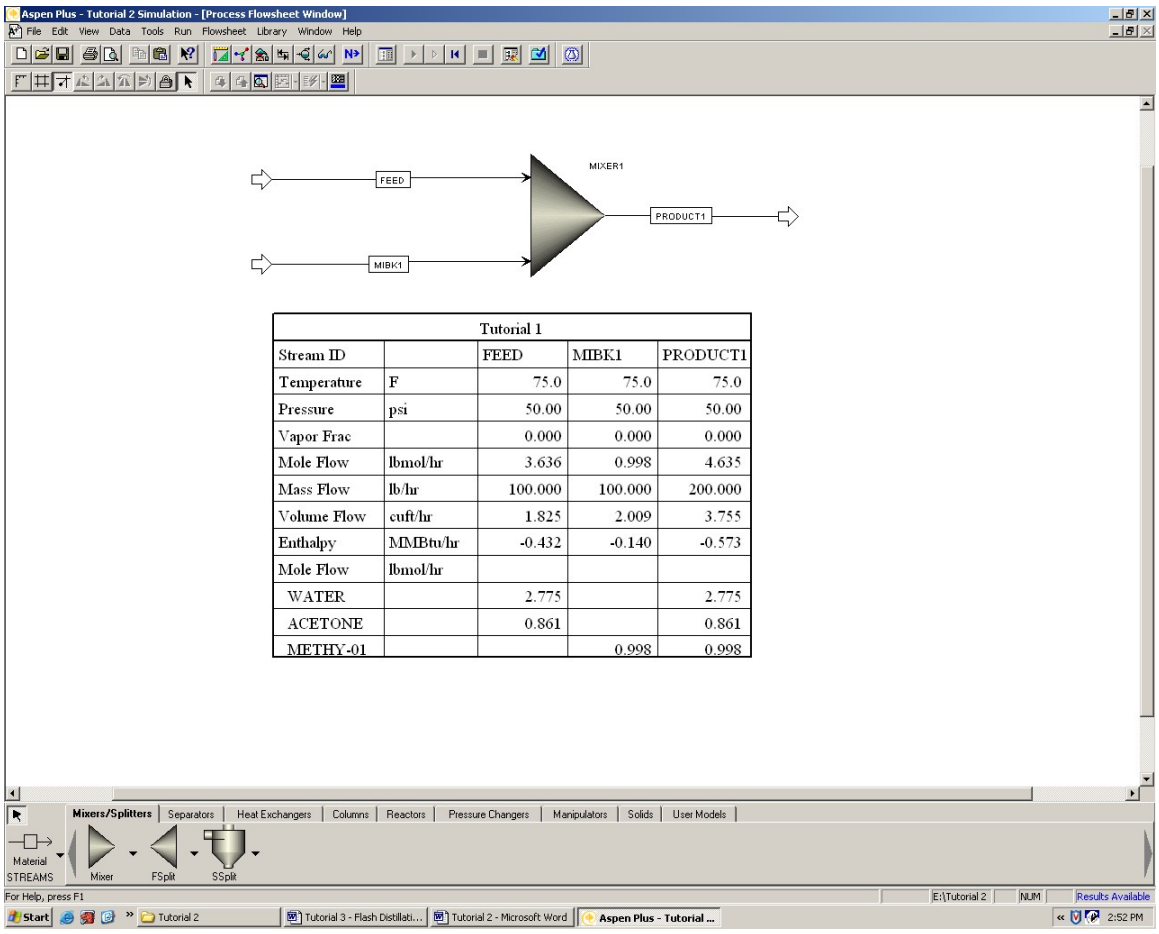


Figure 2: Stream Table Results

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.

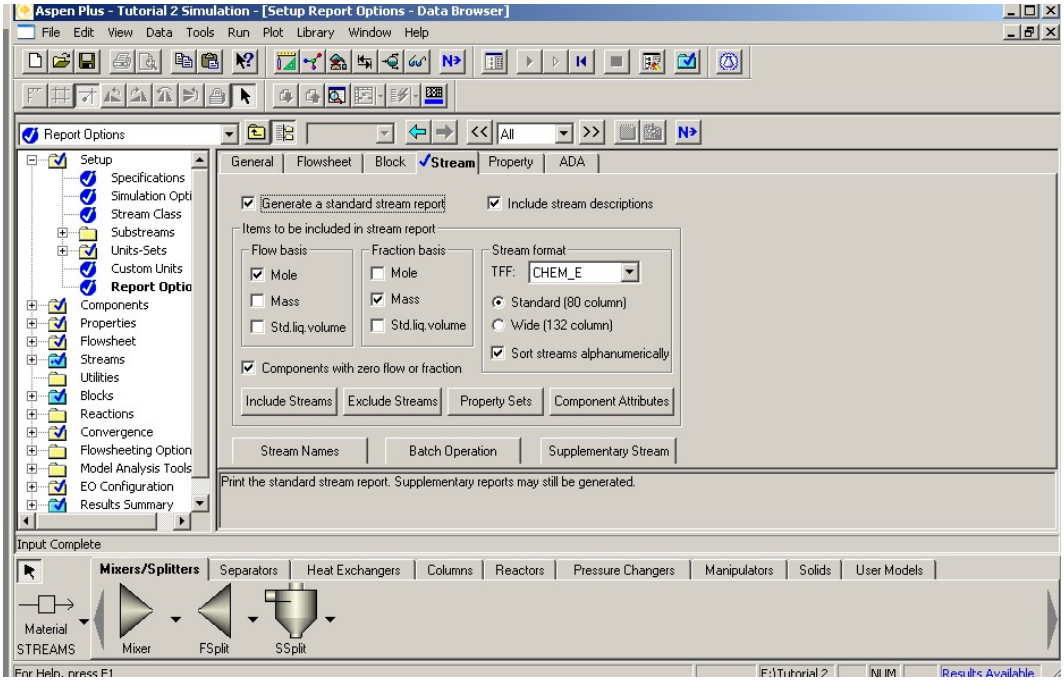
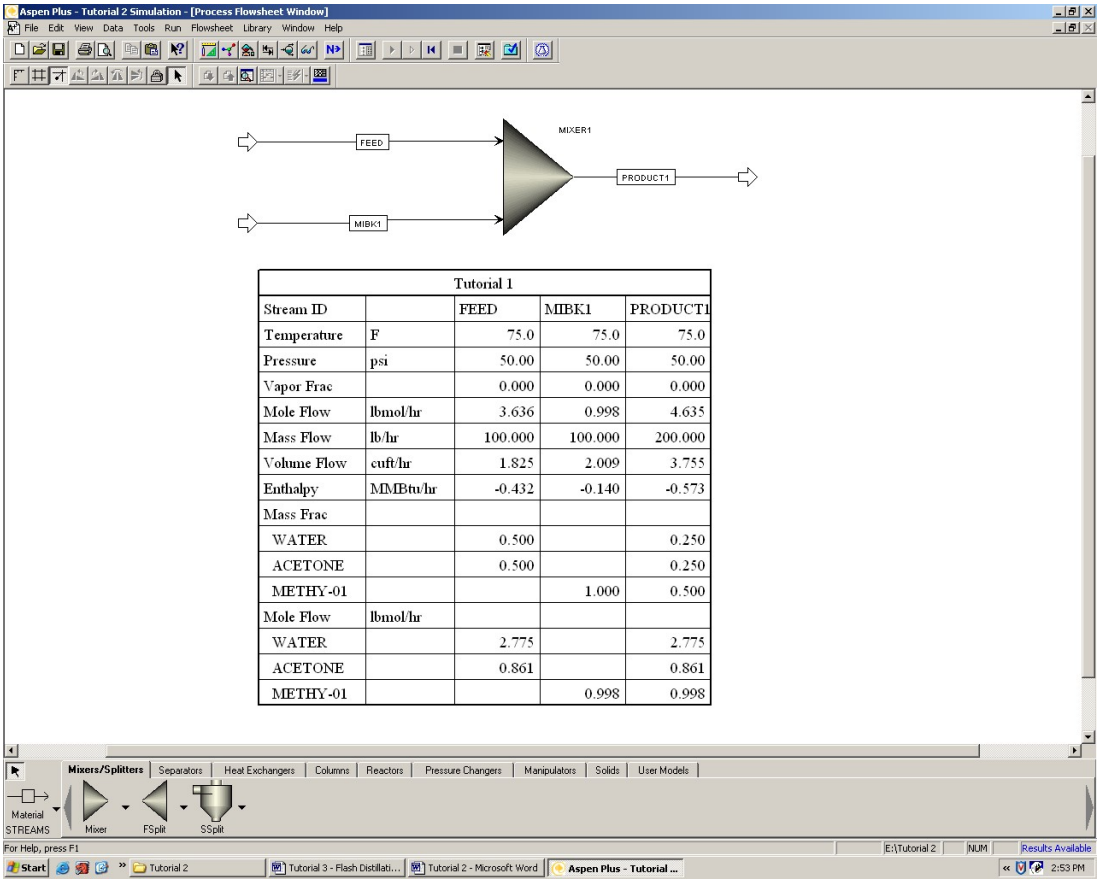


Figure 4: Stream Options



Tutorial 1				
Stream ID		FEED	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 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.

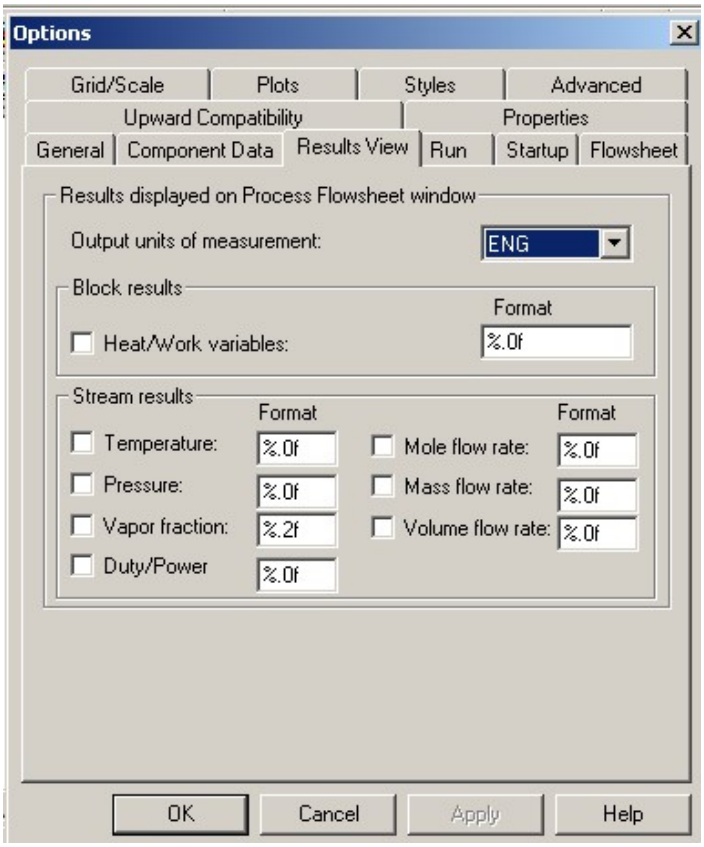
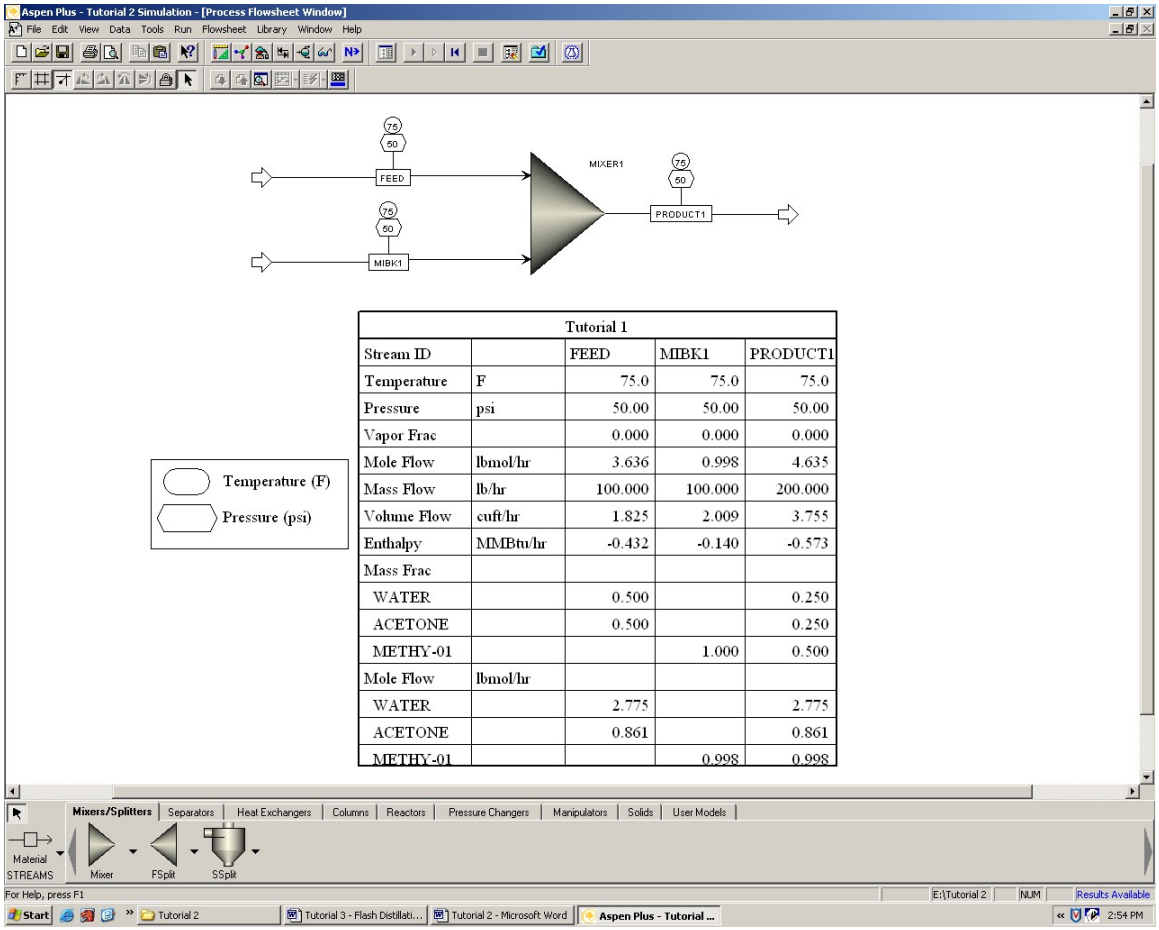


Figure 6: Options Window

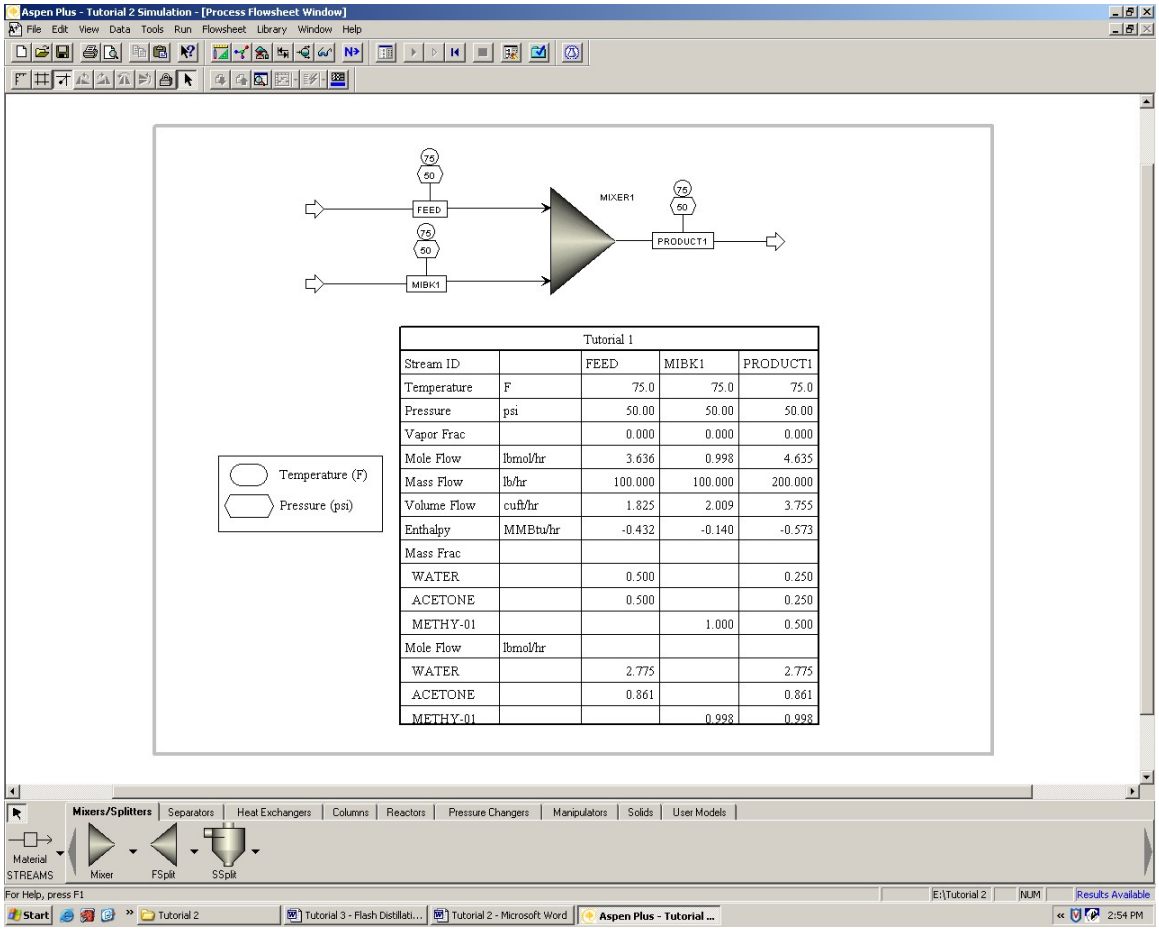


Tutorial 1				
Stream ID		FEED	MIBK1	PRODUCT1
Temperature	F	75.0	75.0	75.0
Pressure	psi	50.00	50.00	50.00
Vapor Frac		0.000	0.000	0.000
Mole Flow	lbmol/hr	3.636	0.998	4.635
Mass Flow	lb/hr	100.000	100.000	200.000
Volume Flow	cuft/hr	1.825	2.009	3.755
Enthalpy	MMBtu/hr	-0.432	-0.140	-0.573
Mass Frac	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



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 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.

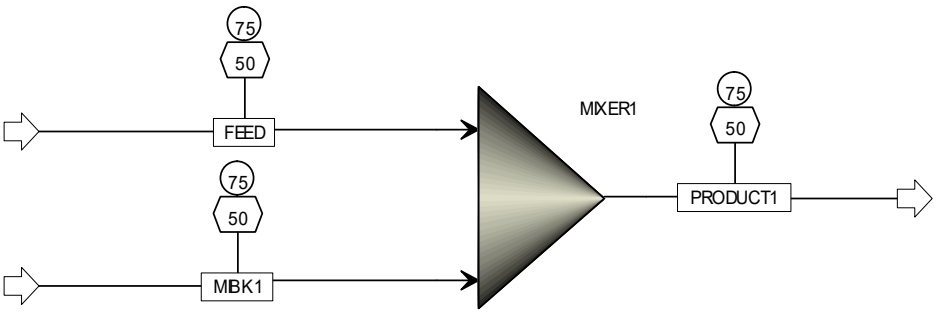
Next week: Flash Distillation

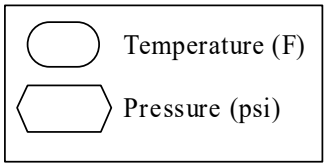
Tutorial #2 Homework and Solution

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
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

```
;
;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
;
;
```

Aspen Tutorial #3: Flash Separation

Outline:

- Problem Description
- Adding a Flash Distillation Unit
- Updating the User Input
- Running the Simulation and Checking the Results
- Generating Txy and Pxy Diagrams

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 building upon our existing simulation by adding a flash separation to our product stream. This unit operation can be used to represent a number of real life pieces of equipment including feed surge drums in refining processes and settlers as in this problem. A flash distillation (or separation) is essentially a one stage separation process and for our problem we are hoping to split our mixture into two streams; one composed of primarily water and acetone and one composed of primarily MIBK and acetone.

Adding a Flash Distillation Unit:

Open up your simulation from last week which you have hopefully saved. Select the Separators tab in the Equipment Model Library and take a minute to familiarize yourself with the different types of separators that are available and their applications as shown in the Status Bar. We will be using a Flash3 separator using a rigorous vapor-liquid-liquid equilibrium to separate our stream for further purification.

Select the Flash3 separator and add one to your process flowsheet. Select the material stream from the stream library and add a product stream leaving the flash separator from the top side, the middle, and the bottom side (where the red arrows indicate a product is required) as shown in Figure 1. Do not add a stream to the feed location yet.

You will notice that I have removed the stream table and stream conditions from my flowsheet from last week. I have done this to reduce the amount of things on the screen and will add them back in at the end of this tutorial. You can leave yours on the process flowsheet while working through this tutorial or you can remove them and add them back in at the end of the tutorial.

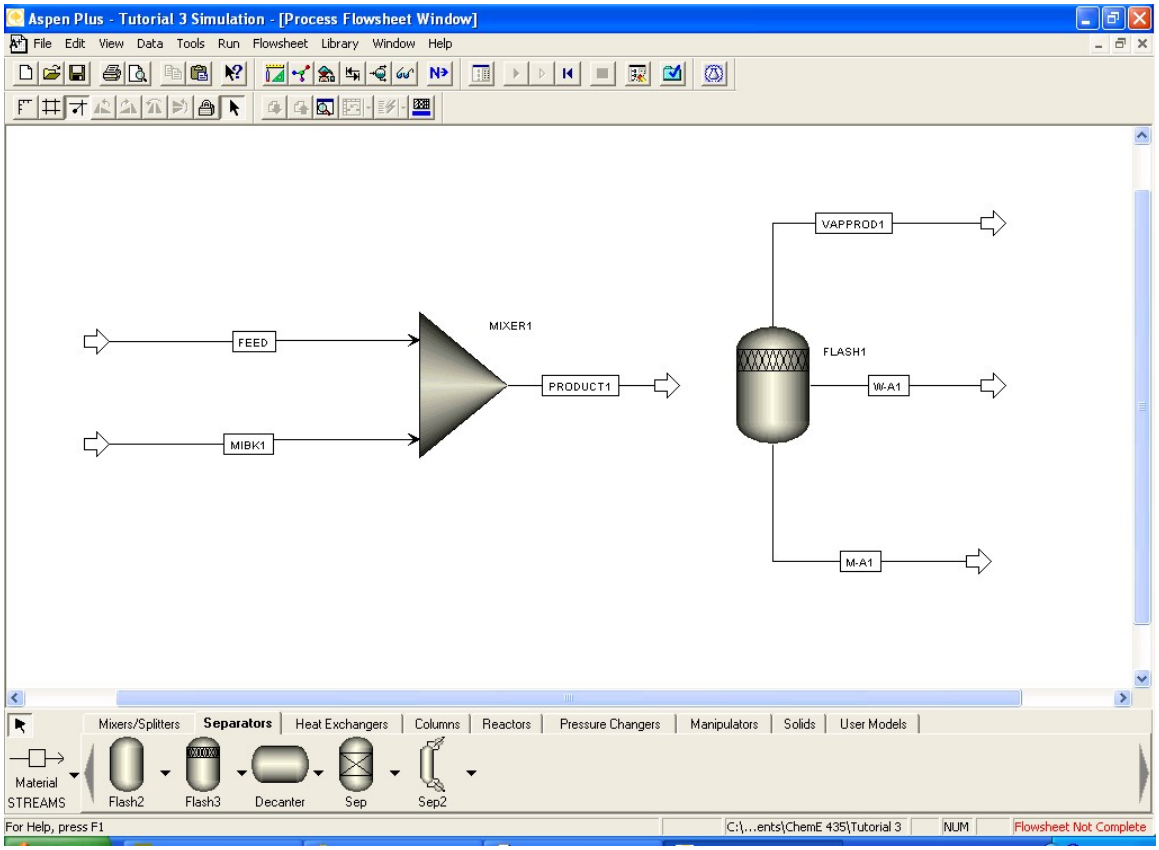


Figure 1: Flash Separator

To connect up the feed stream to your flash separator right click on the product stream from your mixer (mine is named PRODUCT1). Select the option Reconnect Destination and attach this stream to the inlet arrow on the flash separator drum. After renaming your streams as you see fit, your process flowsheet should look similar to that in Figure 2.

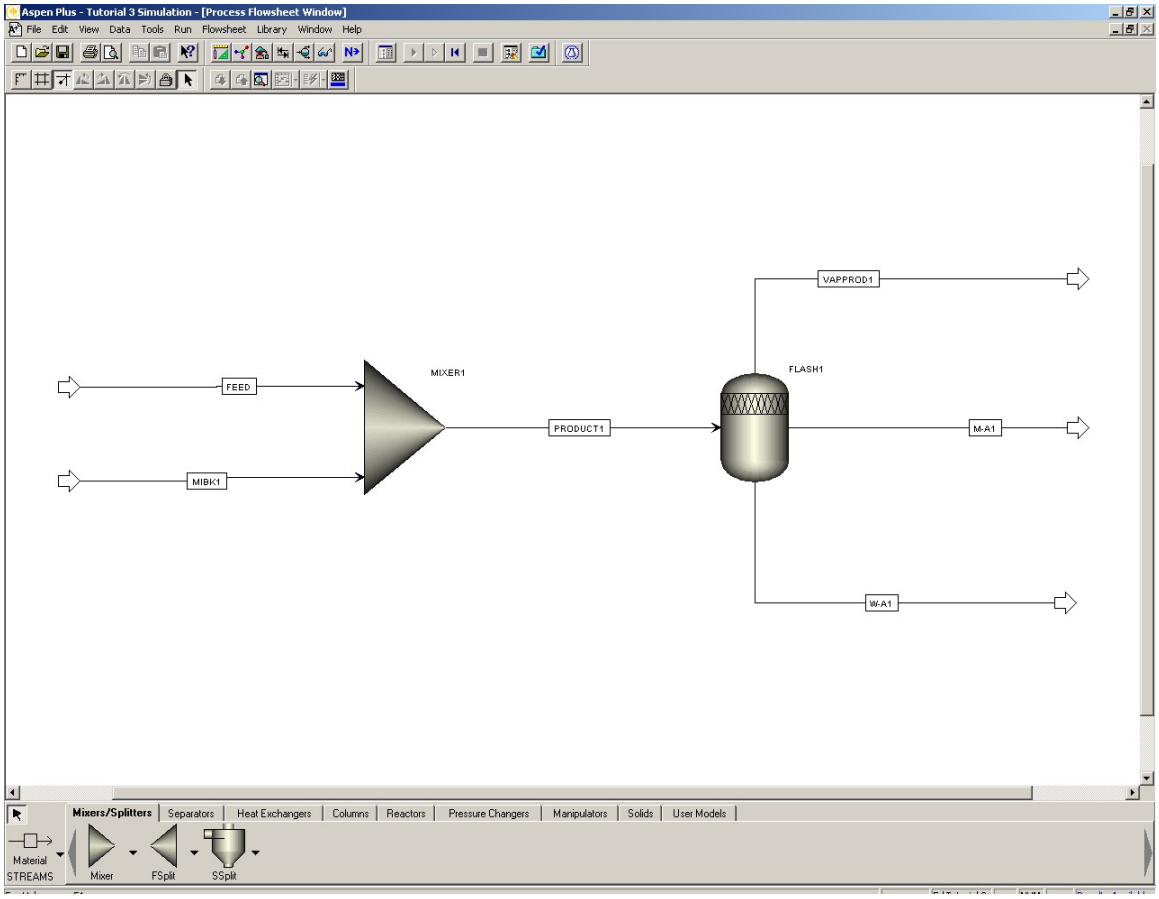


Figure 2: Completed Flowsheet

Updating the User Input:

You will notice that the simulation status has changed to "Required Input Incomplete" because of the new unit operation that we have added to our process flowsheet. When making drastic changes to an existing simulation like we have, it is best to reinitialize the simulation like we did in Tutorial #2. Do so now and then open up the data browser window.

All of the user input is complete except for that in the blocks tab. One of the nice features of Aspen is that you only need to add input data to new feed streams and new equipment and it will complete calculations to determine the compositions for all of the new intermediate and product streams. However, there is one pitfall to this feature. Keep in mind that we originally selected our thermodynamic method based on our original, simpler simulation. Aspen does not force you to go back to the thermodynamic selection to confirm that the user has selected the appropriate thermodynamic base for their problem and this can lead to convergence problems and unrealistic results if it is not considered.

In order for our simulation to properly model VLL equilibrium, we will need to change the thermodynamic method from IDEAL. In the data browser, select specifications under

the Properties tab. Change the Base method from IDEAL to SRK (Soave-Redlich-Kwong equation of state) as shown in Figure 3. Next week we will be discussing the different thermodynamic methods, so this will not be discussed in depth now.

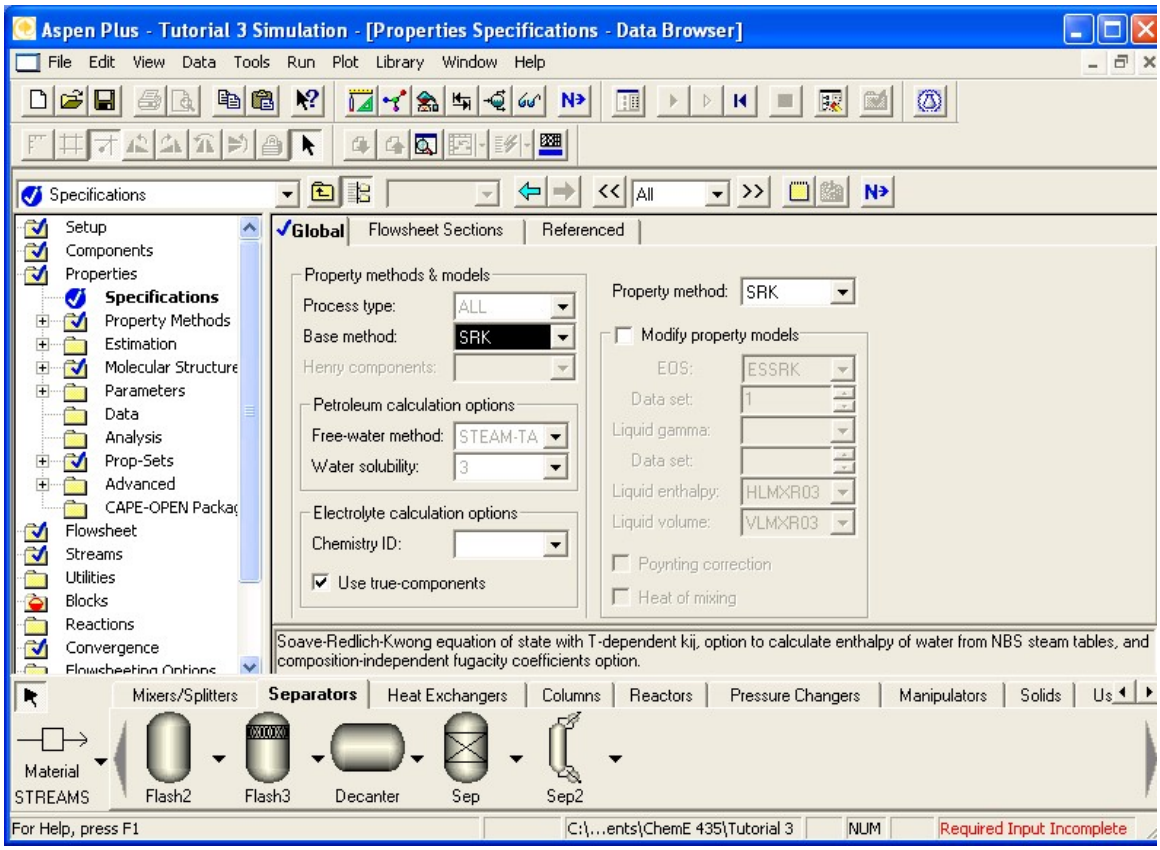


Figure 3: Thermodynamic Base Method

You may notice that the Property method option automatically changes to the SRK method as well. This is fine.

Now open up the Input tab for the FLASH1 block under the blocks tab in the data browser. You will notice that the user can specify two of four variables for the flash separator depending on your particular application. These options are shown in Figure 4. In our simulation we will be specifying the temperature and pressure of our flash separator to be equal to the same values as our feed streams (75º F and 50 psi). After inputting these two values you will notice that the Simulation Status changes to "Required Input Complete".

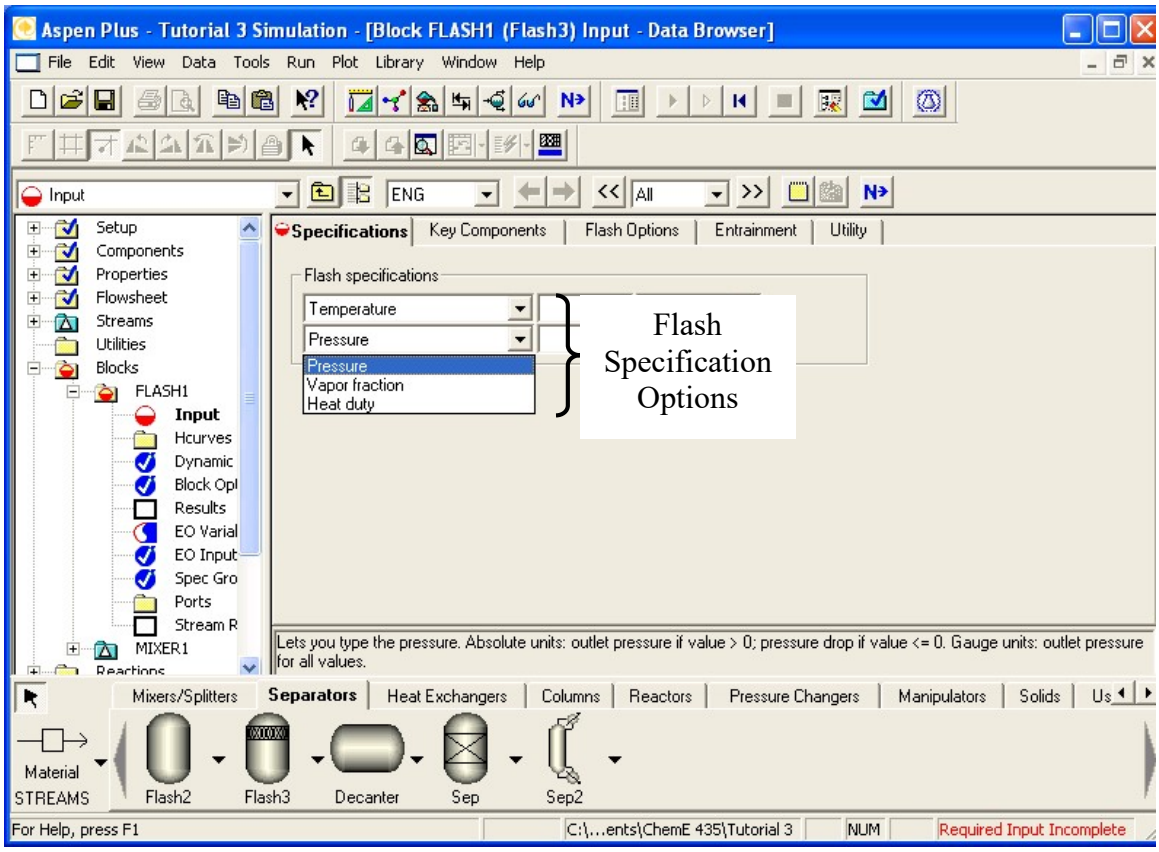
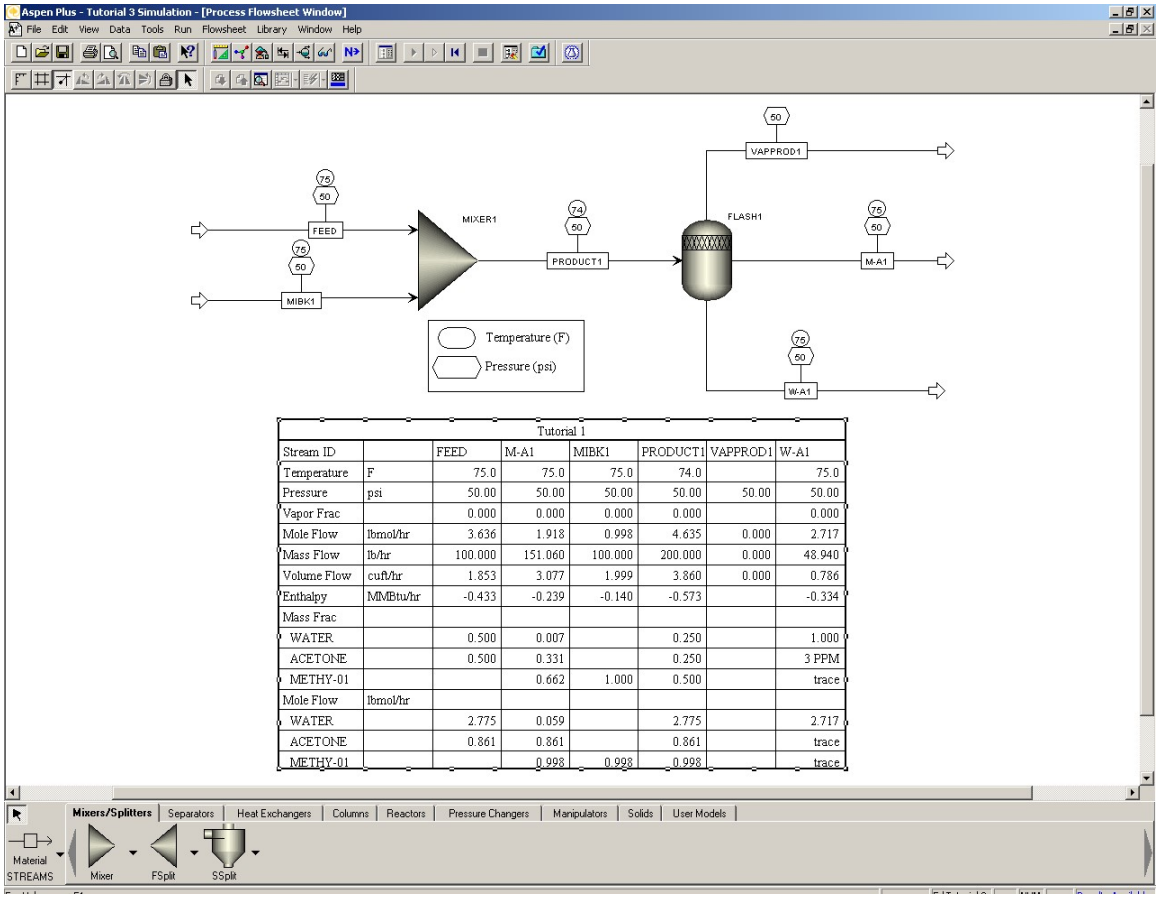


Figure 4: Flash Data Input Options

Running the Simulation and Checking the Results:

Run your simulation at this time. As in tutorial #2, be sure to check your results for both convergence and run status. In doing so you will notice a system warning that arises due to changes in the simulation that we have made. Follow the suggestions presented by Aspen and change to the STEAMNBS method as recommended (Hint: the change is under the properties tab). Reinitialize and rerun your simulation after making this change.

At this point your process flowsheet should look like that seen in Figure 5 (as mentioned earlier I have now placed the stream table and process flow conditions back onto my flowsheet).



Tutorial 1

Stream ID		FEED	M-A1	MIBK1	PRODUCT1	VAPPROD1	W-A1
Temperature	F	75.0	75.0	75.0	74.0		75.0
Pressure	psi	50.00	50.00	50.00	50.00	50.00	50.00
Vapor Frac		0.000	0.000	0.000	0.000		0.000
Mole Flow	lbmol/hr	3.636	1.918	0.998	4.635	0.000	2.717
Mass Flow	lb/hr	100.000	151.060	100.000	200.000	0.000	48.940
Volume Flow	cuft/hr	1.853	3.077	1.999	3.860	0.000	0.786
Enthalpy	MMBtu/hr	-0.433	-0.239	-0.140	-0.573		-0.334
Mass Frac							
WATER		0.500	0.007		0.250		1.000
ACETONE		0.500	0.331		0.250		3 PPM
METHY-01			0.662	1.000	0.500		trace
Mole Flow	lbmol/hr						
WATER		2.775	0.059		2.775		2.717
ACETONE		0.861	0.861		0.861		trace
METHY-01			0.998	0.998	0.998		trace

Figure 5: Completed Process Flowsheet

Due to the added clutter on the screen I would recommend removing the process flow conditions at this time. These values are available in the stream table and do not provide much added benefit for our application.

You will notice that our simulation results in nearly perfect separation of the water from the MIBK and acetone mixture. However, in real life this mixture is not this easy to separate. This simulation result is directly caused by the thermodynamic methods we have selected and you will see the influence that thermodynamics play in the tutorial next week.

Generating Txy and Pxy Diagrams:

Aspen and other simulation programs are essentially a huge thermodynamic and physical property data bases. We will illustrate this fact by generating a Txy plot for our acetone-MIBK stream for use in specifying our distillation column in a few weeks. In the menu bar select Tools/Analysis/Property/Binary. When you have done this the Binary Analysis window will open up as shown in Figure 6.

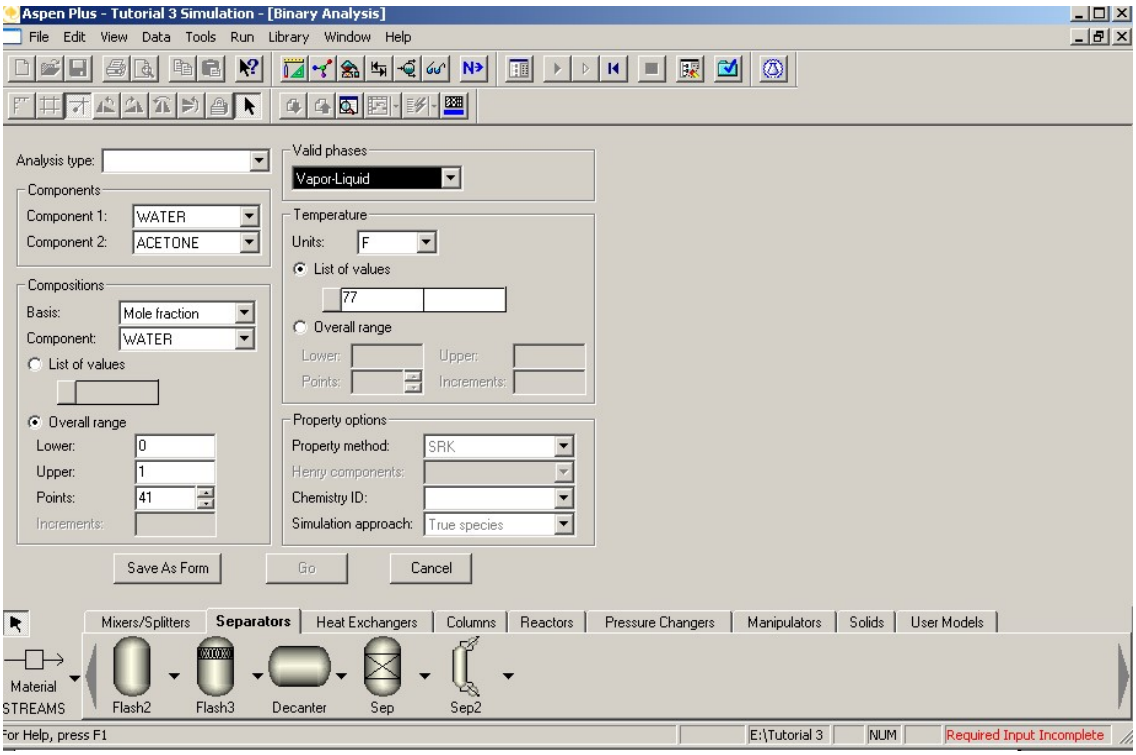


Figure 6: Binary Analysis Window

You will notice that this option can be used to generate Txy, Pxy, or Gibbs energy of mixing diagrams. Select the Txy analysis. You also have the option to complete this analysis for any of the components that have been specified in your simulation. We will be doing an analysis on the mixture of MIBK and acetone so select these components accordingly. In doing an analysis of this type the user also has the option of specifying which component will be used for the x-axis (which component's mole fraction will be diagrammed). The default is whichever component is indicated as component 1. Make sure that you are creating the diagram for the mole fraction of MIBK. When you have completed your input, hit the go button on the bottom of the window.

When you select this button the Txy plot will appear on your screen as shown in Figure 7. The binary analysis window will open up behind this plot automatically as well (we will get to that window in a minute).

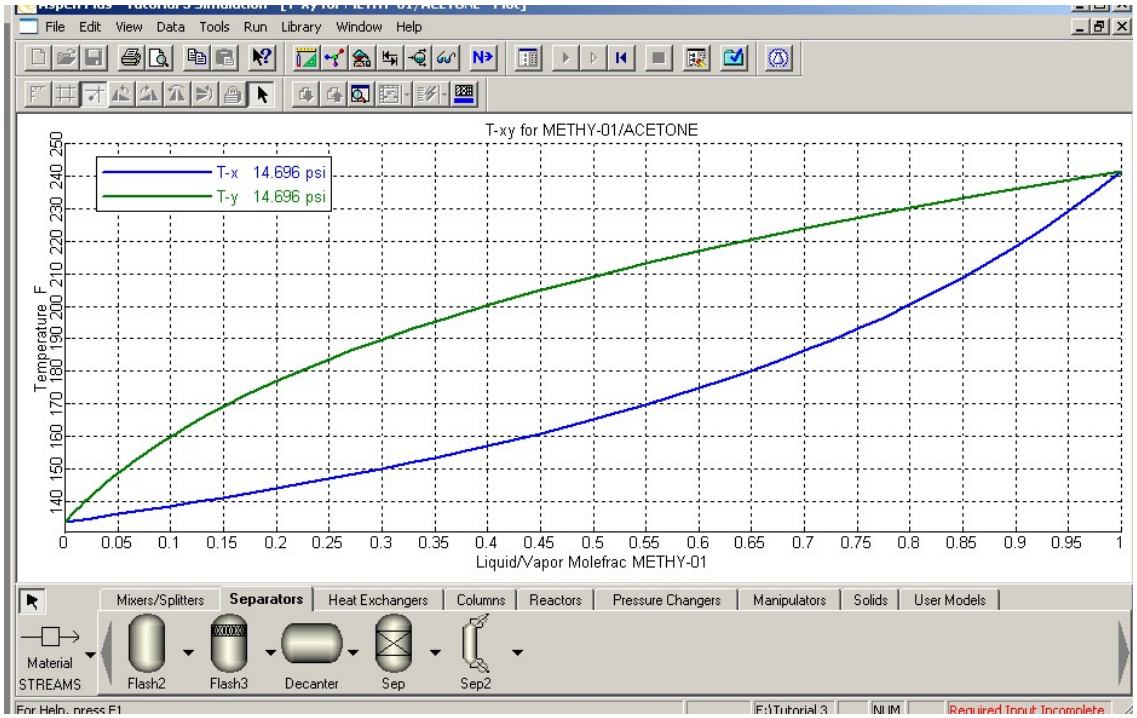


Figure 7: Txy Plot for MIBK and Acetone

The plot window can be edited by right clicking on the plot window and selecting properties. In the properties window the user can modify the titles, axis scales, font, and color of the plot. The plot window can also be printed directly from Aspen by hitting the print key.

Close the plot window at this point in time. The binary analysis results window should now be shown on your screen. This window is shown in Figure 8. You can see that this window shows a large table of thermodynamic data for our two selected components. We can use this data to plot a number of different things using the plot wizard button at the bottom of the screen. Select that button now.

In step 2 of the plot wizard you are presented with five options for variables that you can plot for this system. Gamma represents the liquid activity coefficient for the components and it is plotted against mole fraction. The remainder of the plot wizard allows you to select the component and modify some of the features of the plot that you are creating and upon hitting the finish button, your selected plot should open. Again, the plot can be further edited by right-clicking on the plot and selecting properties. In the homework for this week you will be turning in a plot of the liquid activity coefficient, so you can do that now if you would like. Otherwise, you can save your simulation for next week when we examine the various thermodynamic methods used by Aspen.

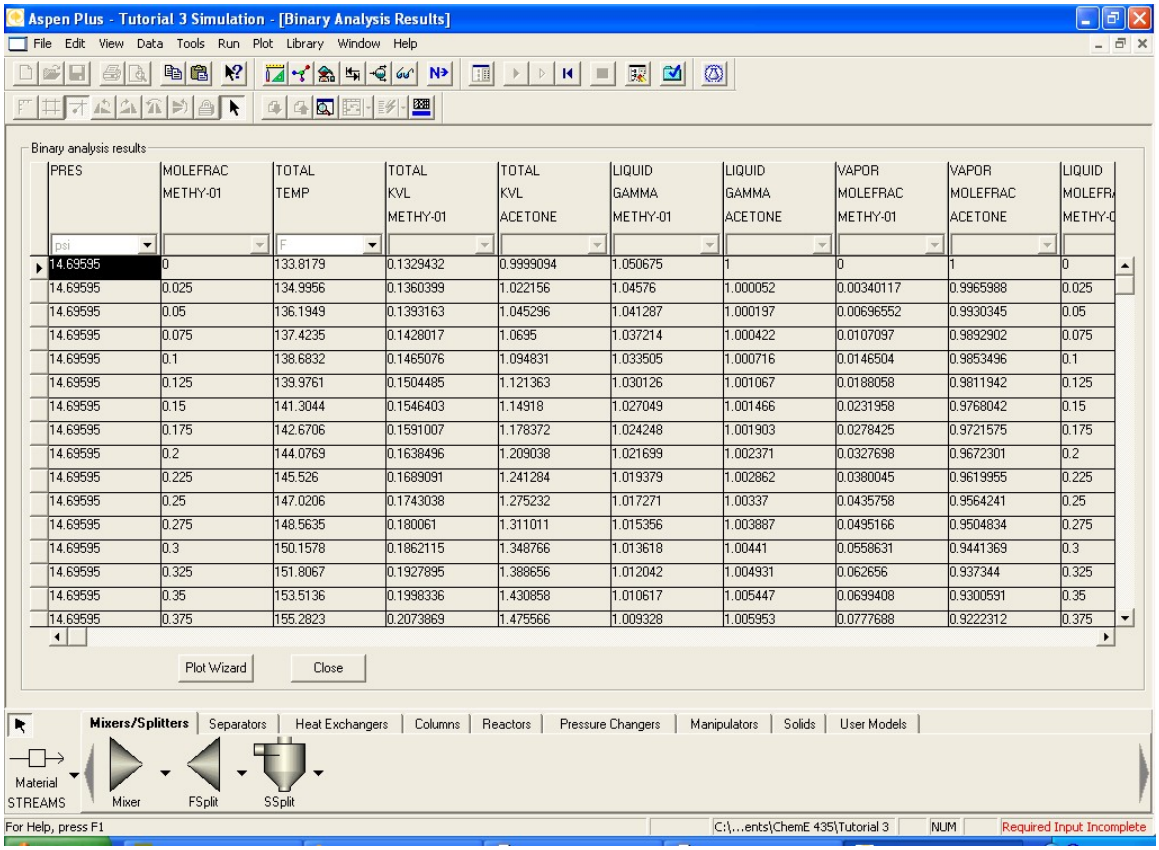


Figure 8: Binary Analysis Results Window

Next week: Thermodynamic Methods

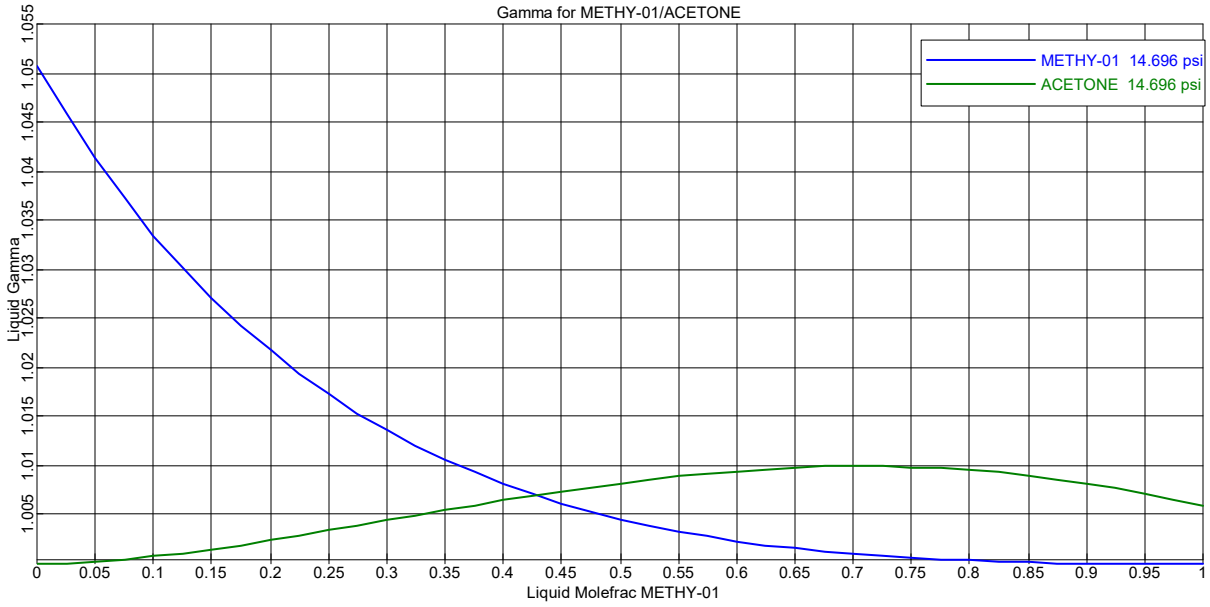
Tutorial #3 Homework and Solution

Question:

a) Provide a copy of the complete stream table developed in Tutorial #3 showing the composition of the three product streams resulting from your flash separation. Hint: You can select the table in the process flowsheet and copy and paste it into a word document if you would like.
b) Print out and turn in a copy of the plot for the liquid activity coefficient for the MIBK/acetone system (Hint: gamma).

Solution:

Tutorial1							
Stream ID		FEED	M-A1	MIBK1	PRODUCT1	VAPPROD1	W-A1
Temperature	F	75.0	75.0	75.0	74.0		75.0
Pressure	psi	50.00	50.00	50.00	50.00	50.00	50.00
Vapor Frac		0.000	0.000	0.000	0.000		0.000
Mole Flow	lbmol/hr	3.636	1.918	0.998	4.635	0.000	2.717
Mass Flow	lb/hr	100.000	151.060	100.000	200.000	0.000	48.940
Volume Flow	cuft/hr	1.853	3.077	1.999	3.860	0.000	0.786
Enthalpy	MMBtu/hr	-0.433	-0.239	-0.140	-0.573		-0.334
Mass Frac							
WATER		0.500	0.007		0.250		1.000
ACETONE		0.500	0.331		0.250		3 PPM
METHY-01			0.662	1.000	0.500		trace
Mole Flow	lbmol/hr						
WATER		2.775	0.059		2.775		2.717
ACETONE		0.861	0.861		0.861		trace
METHY-01			0.998	0.998	0.998		trace


Gamma for METHY-01/ACETONE
METHY-01 14.696 psi
ACETONE 14.696 psi
Liquid Gamma
1.055
1.05
1.045
1.04
1.035
1.03
1.025
1.02
1.015
1.01
1.005
0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.4
0.45
0.5
0.55
0.6
0.65
0.7
0.75
0.8
0.85
0.9
0.95
1
Liquid Molefrac METHY-01