University of Washington

Department of Chemical Engineering

ASPEN PLUS 12.1 Instructional Tutorials

Developed in the Fall Quarter of 2004

in Chem E 435 (Mass Transfer and Separation)

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This Tutorial was developed with the Windows Version of *ASPEN PLUS 12.1*. Our Site License allows us to install a software version on the personal computer of the instructor and TA. The Tutorial was developed with the idea in mind that it is used and extended in other courses of the ChemE Curriculum. As it currently stands, the tutorial is applicable for students in:

ChemE 310 (Unit Operations): Tutorial Units 1-3,

ChemE 326 (Thermodynamics): Tutorial Units 4 and 5,

ChemE 435 (Mass Transfer and Separations): Tutorial Units 3-6.

Additional unit developments are suggested for:

- Chemical Reactions (ChemE 465)
- Chemical Reactor Design (ChemE 465)
- Heat Streams (ChemE 340 / ChemE 435)
- Heat Exchanger Design (ChemE 340)
- Pressure Drop Calculations (pipe, pumps, valves, etc.) (ChemE 330)
- Using Fortran Statements (ChemE 465)

The ASPEN 10.1 Tutorial developed in ChemE 310 by Martin and Babb would provide some background information on Fortran Statements, Chemical Reactions and Heat Streams and Heat Exchanger Design.

A fast printable PDF version of this Tutorial and a MS-Word version for further unit developments and improvements can be downloaded at

http://courses.washington.edu/overney/ChemE435.html.

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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.

Aspen Tutorial #1

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.
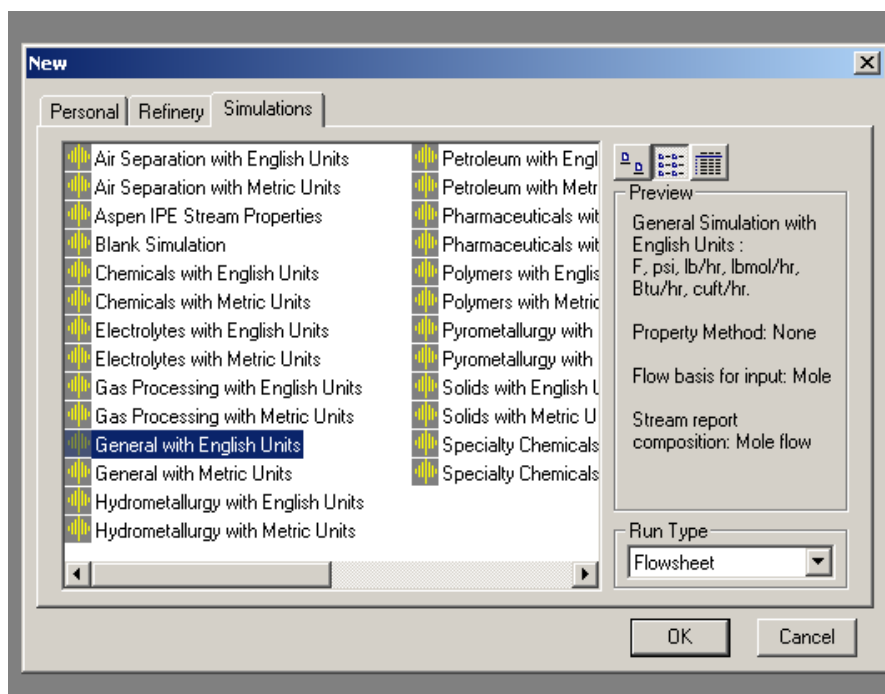

Figure 1: Available Simulation Templates

   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.

Aspen Tutorial #1

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.
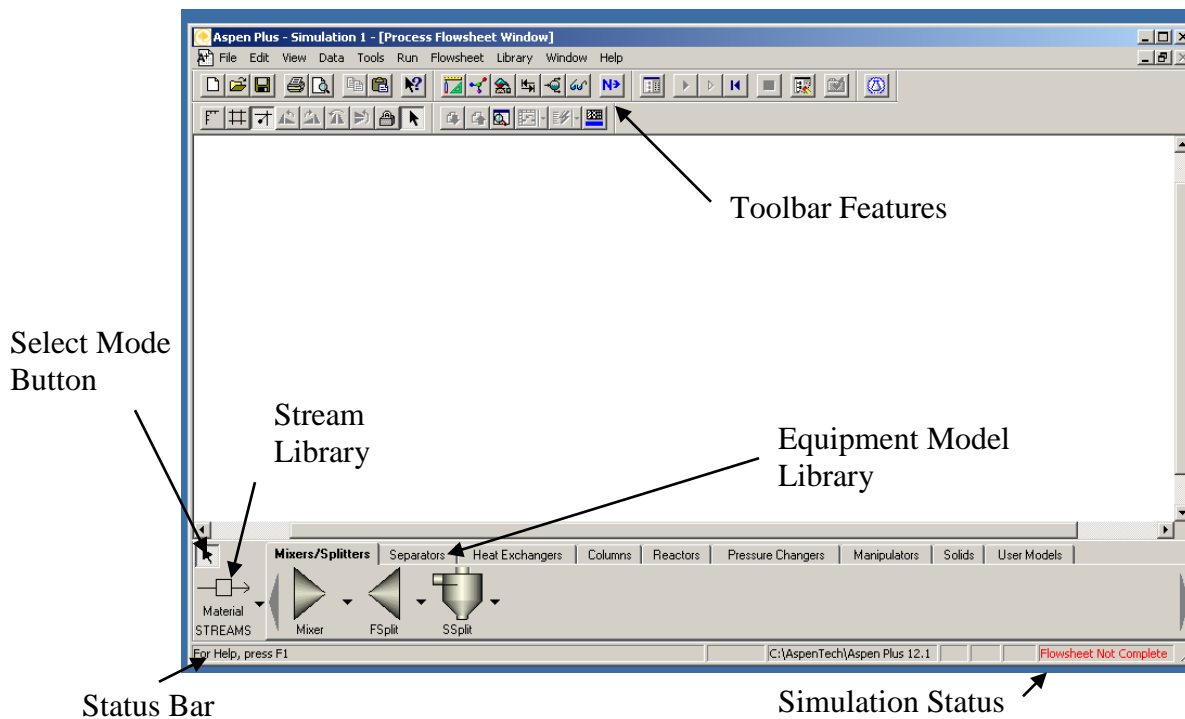

Figure 2: Process Flowsheet Window

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.
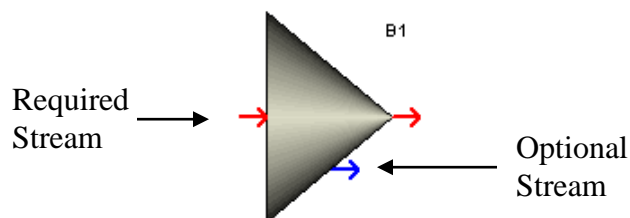

Figure 3: Required Stream Locations

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".
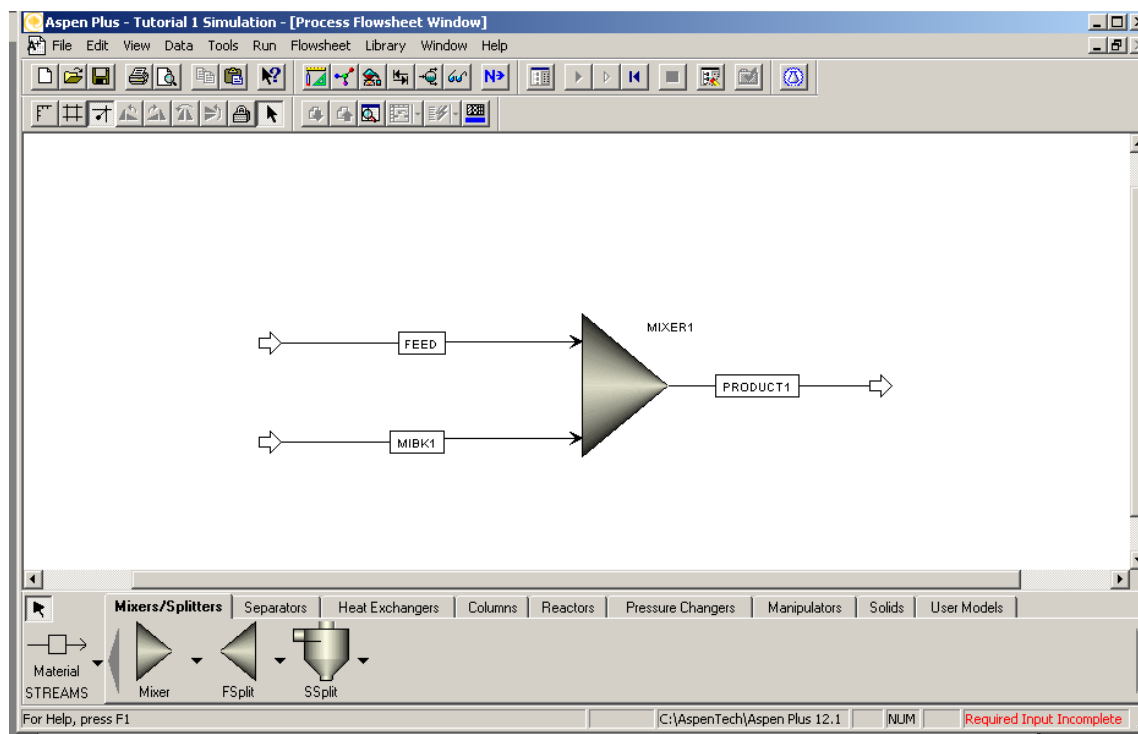
Aspen Tutorial #1

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.
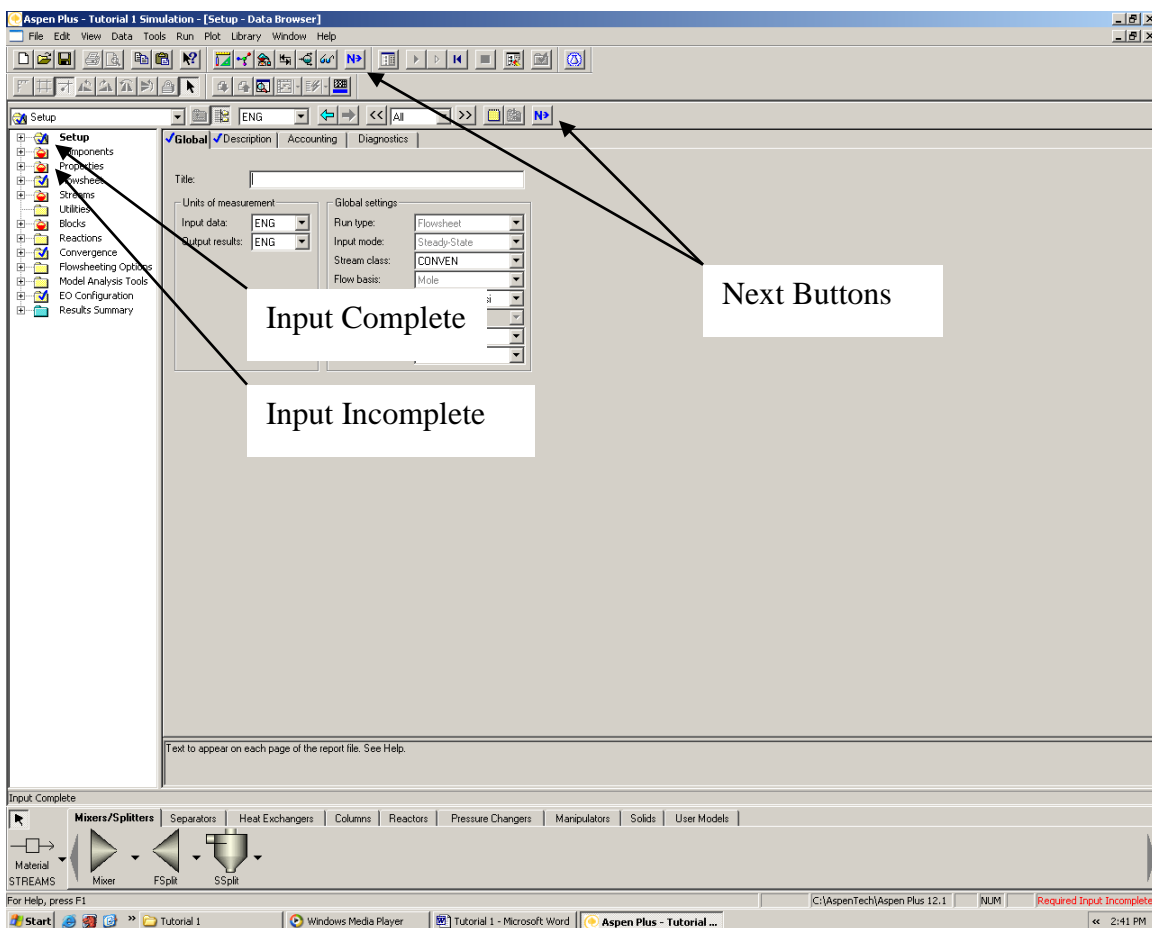
Aspen Tutorial #1

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).

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Aspen Tutorial #1

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.
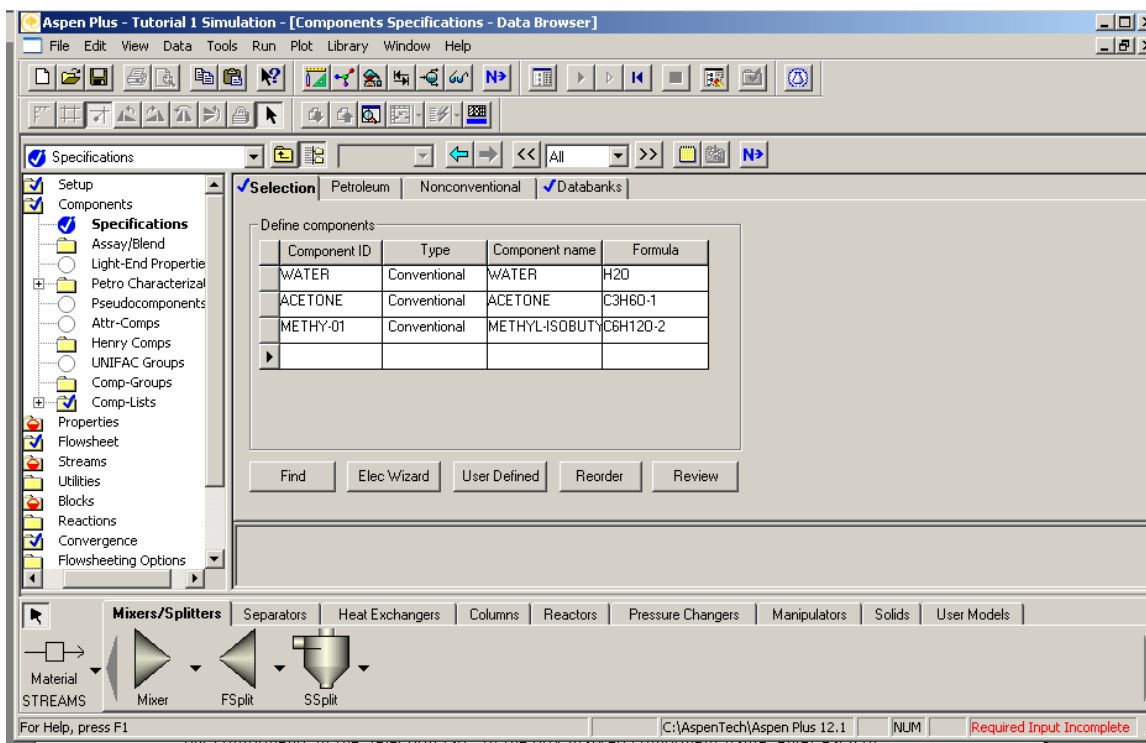

Figure 6: Component Selection

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.
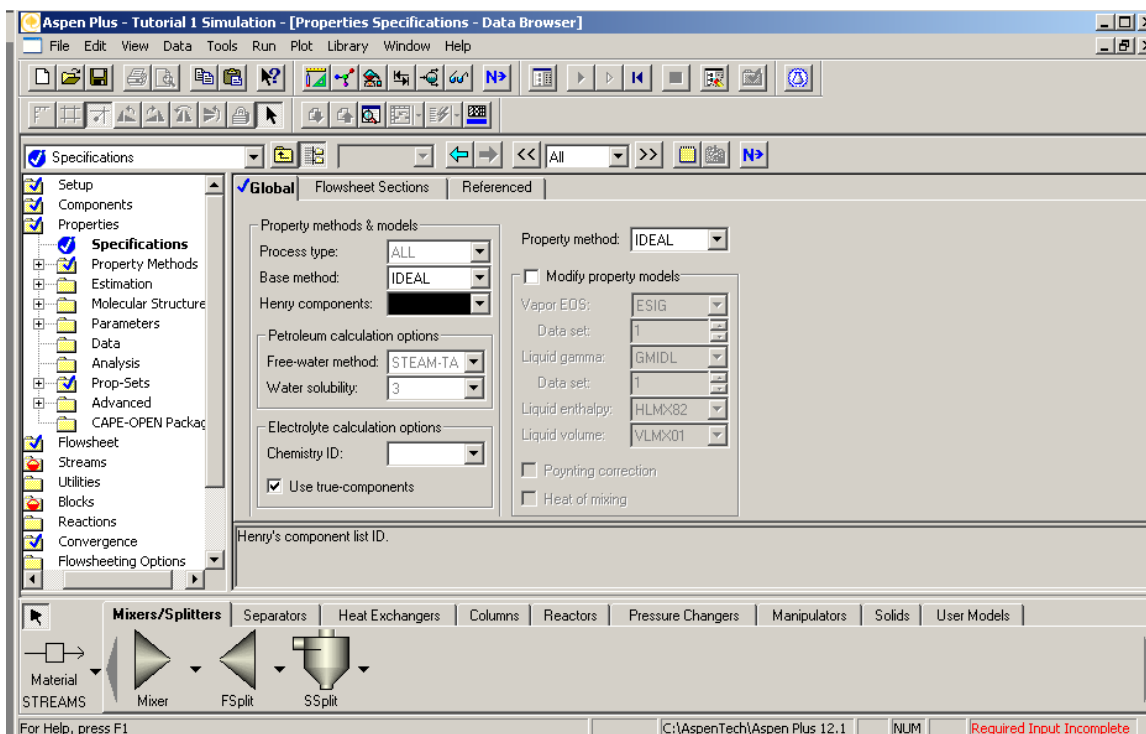
Aspen Tutorial #1

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.
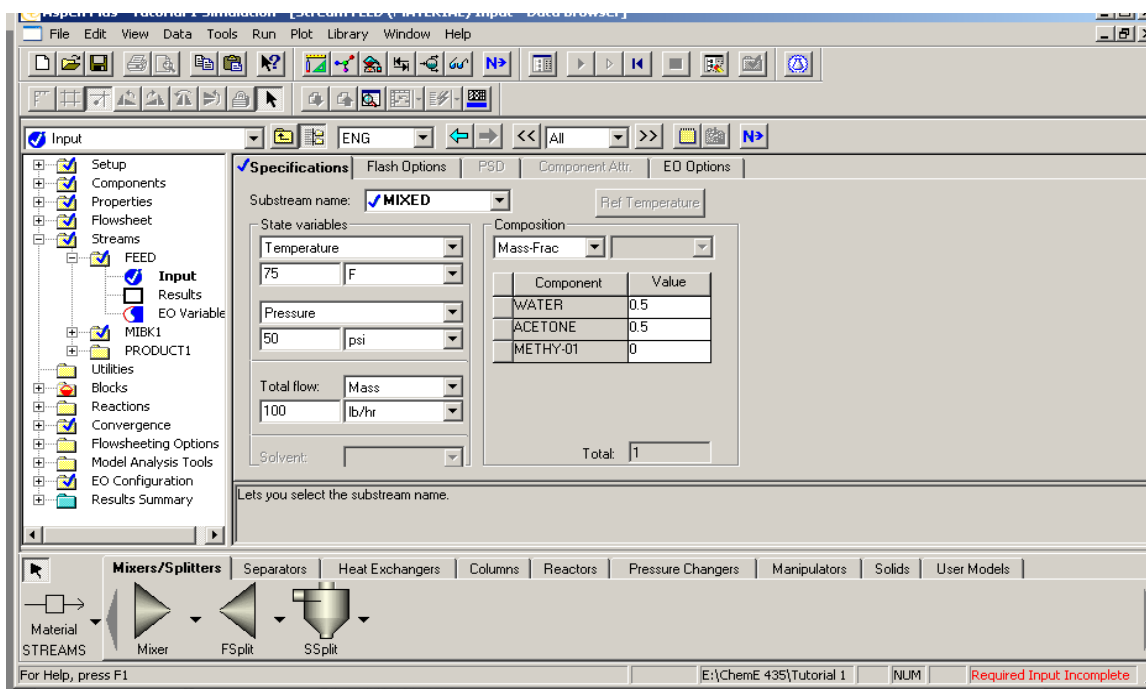
Aspen Tutorial #1

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.
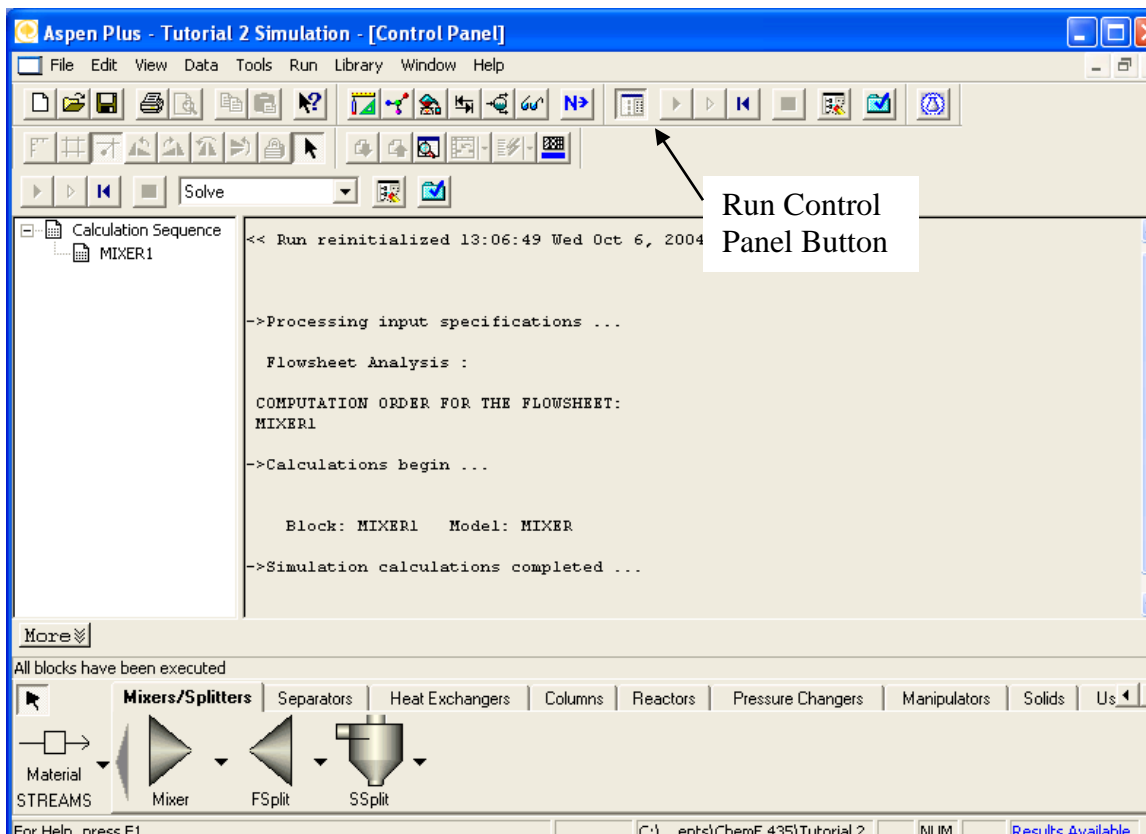

Figure 1: Convergence Status Window

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.

Aspen Tutorial #2

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.
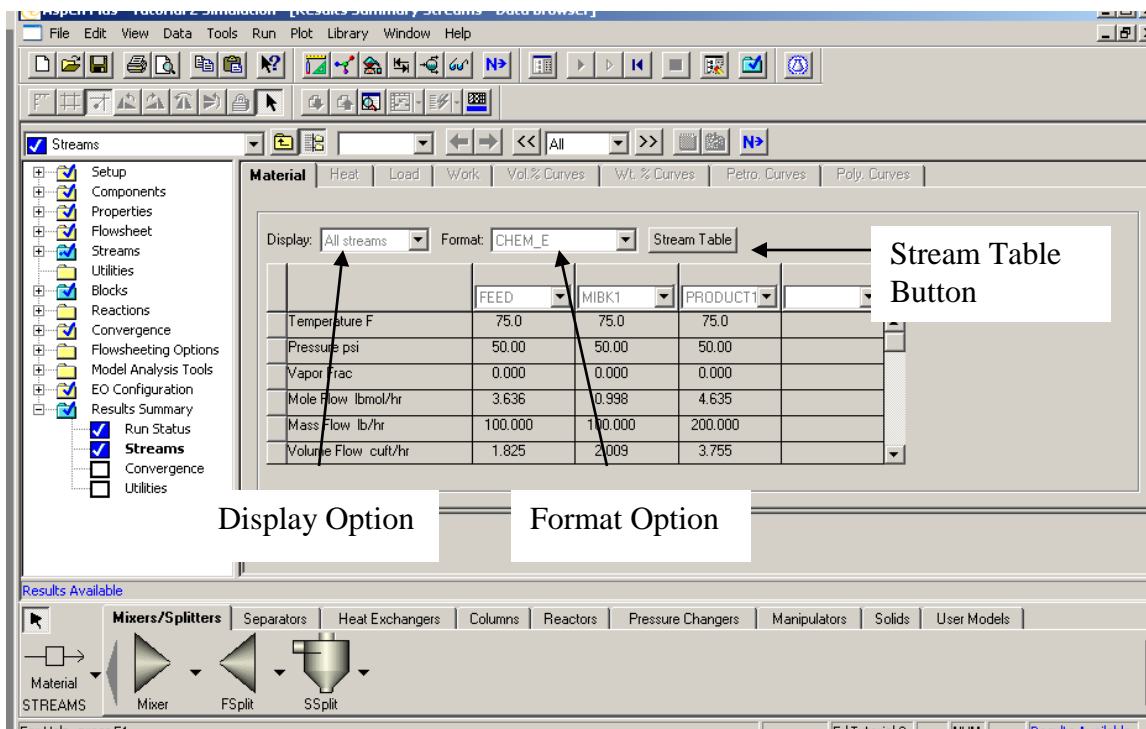

Figure 2: Stream Table Results

After you have added a stream table your process flowsheet should look similar to that seen in Figure 3.
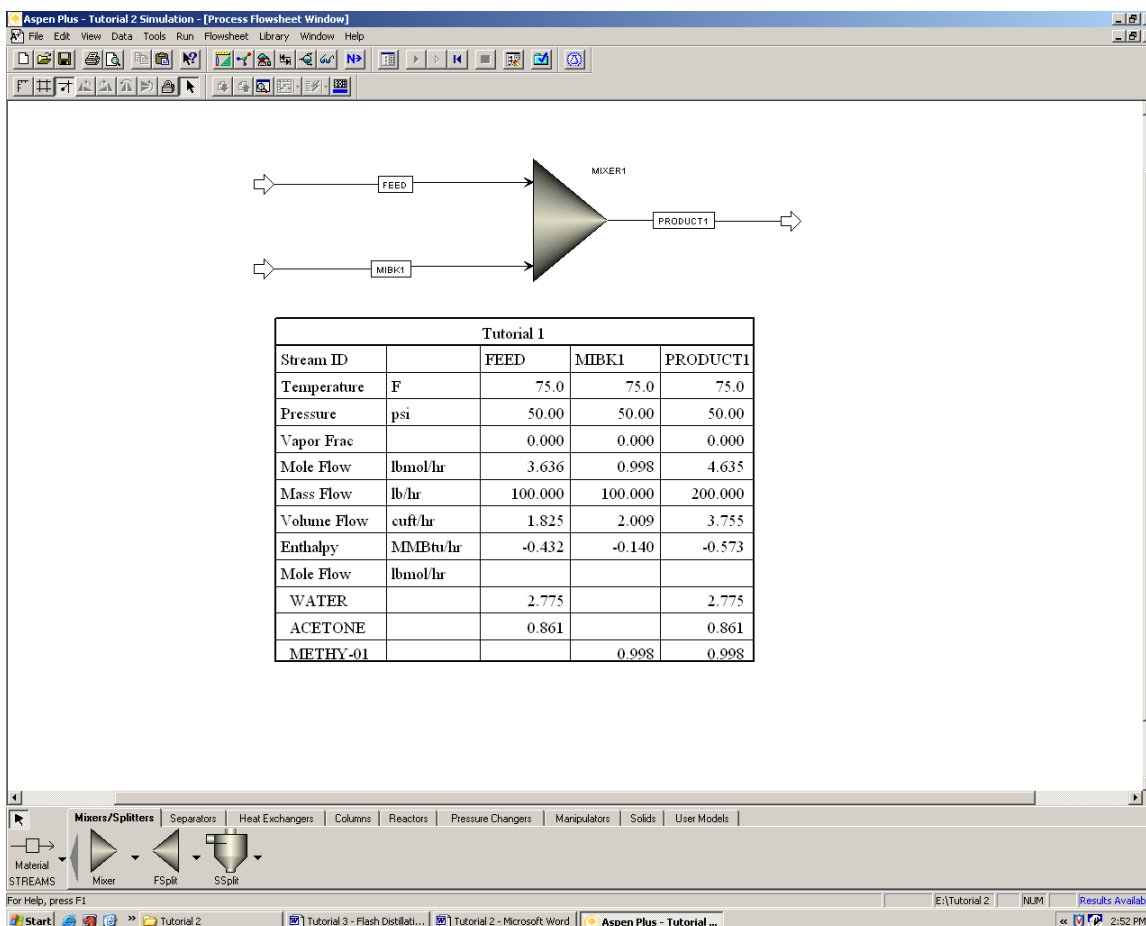
Aspen Tutorial #2

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.

Aspen Tutorial #2
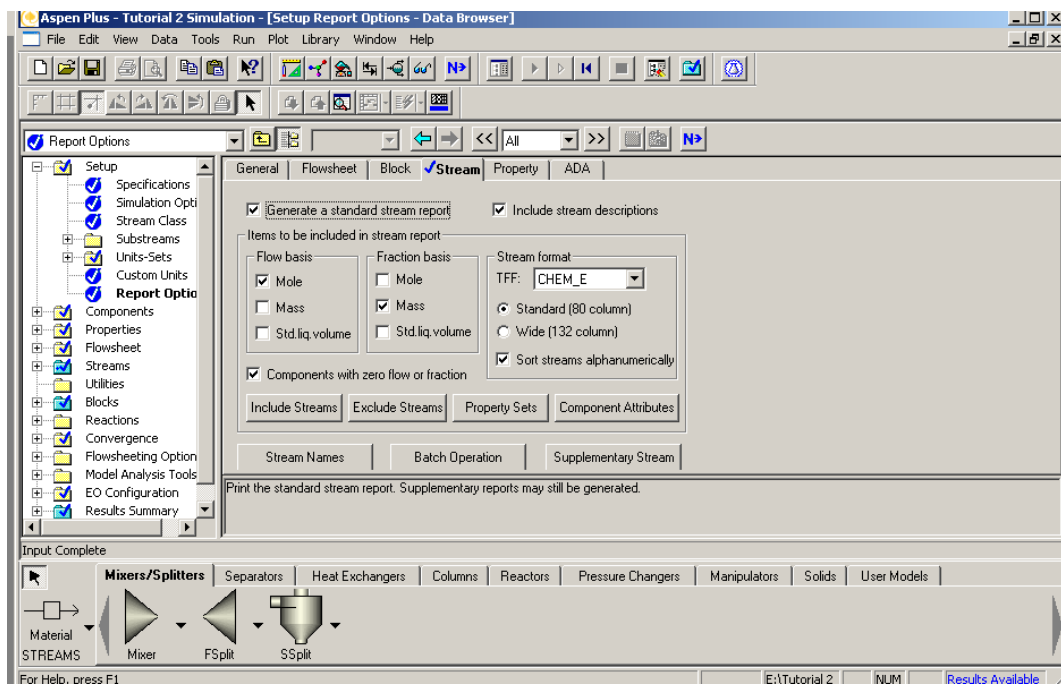
Figure 4: Stream Options
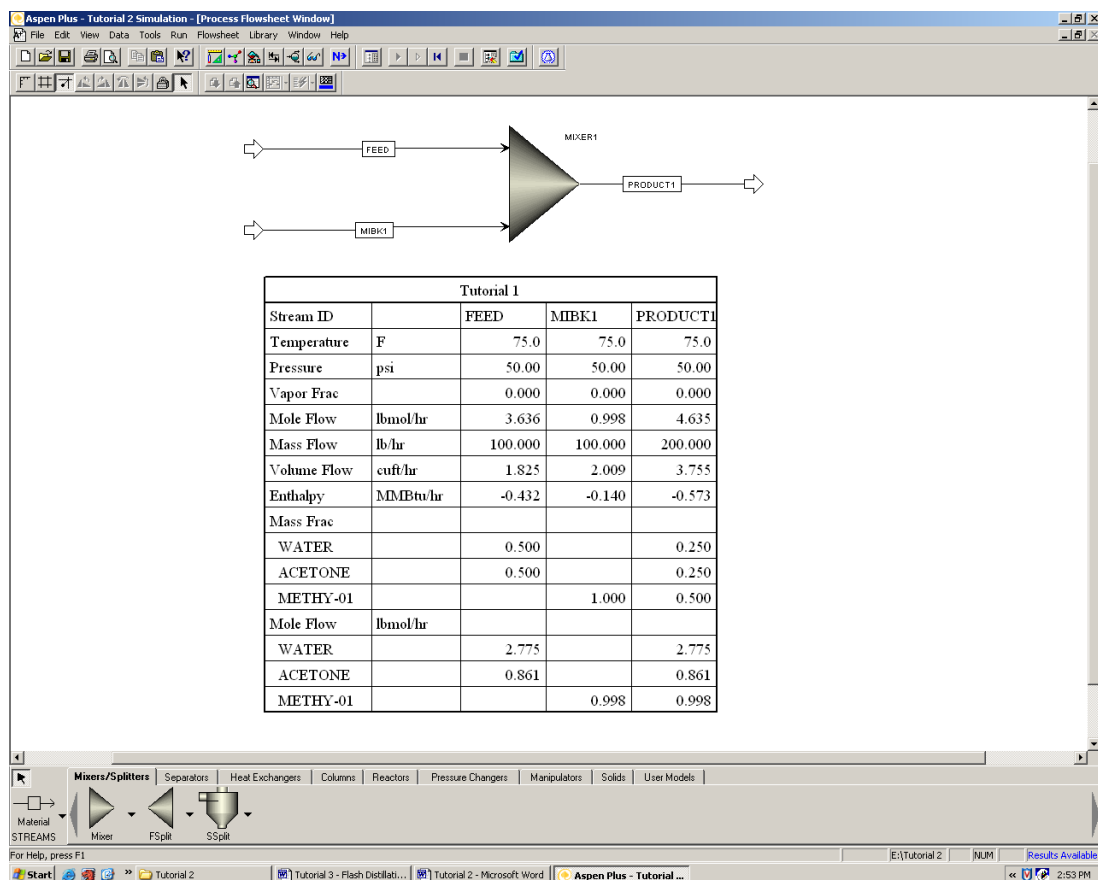
Figure 5: Updated Stream Table

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.
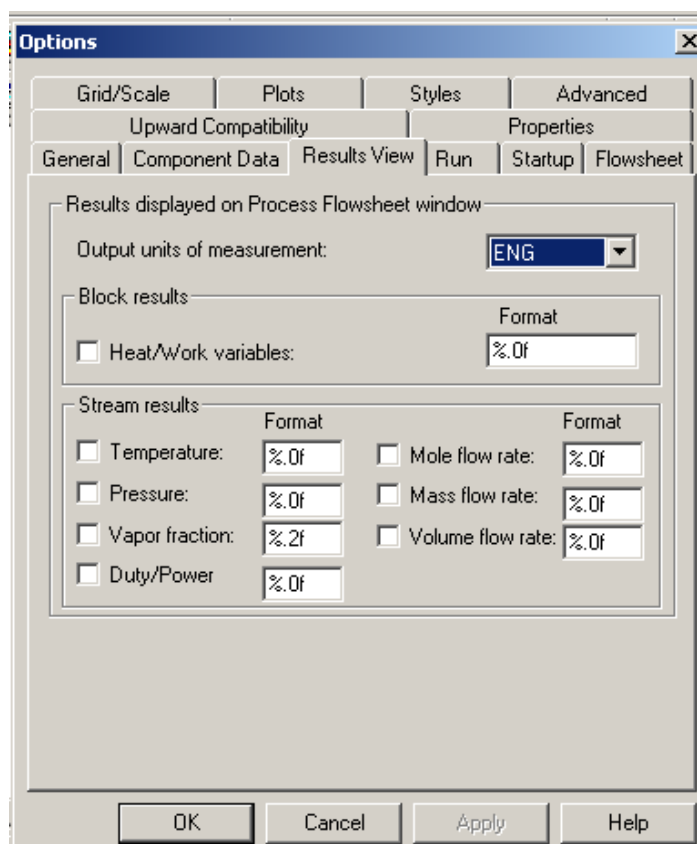
Figure 6: Options Window

Aspen Tutorial #2
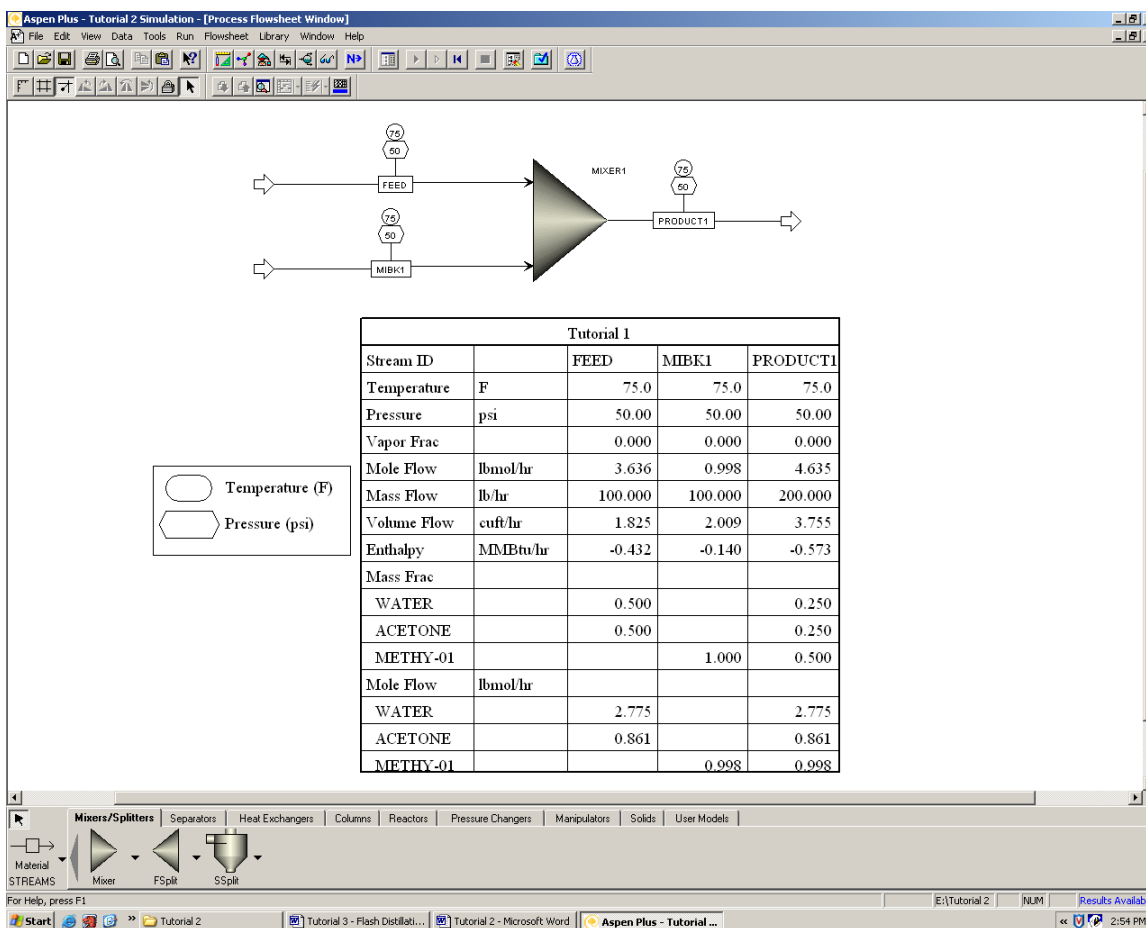
Figure 7: Updated Process Flowsheet

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.

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Aspen Tutorial #2
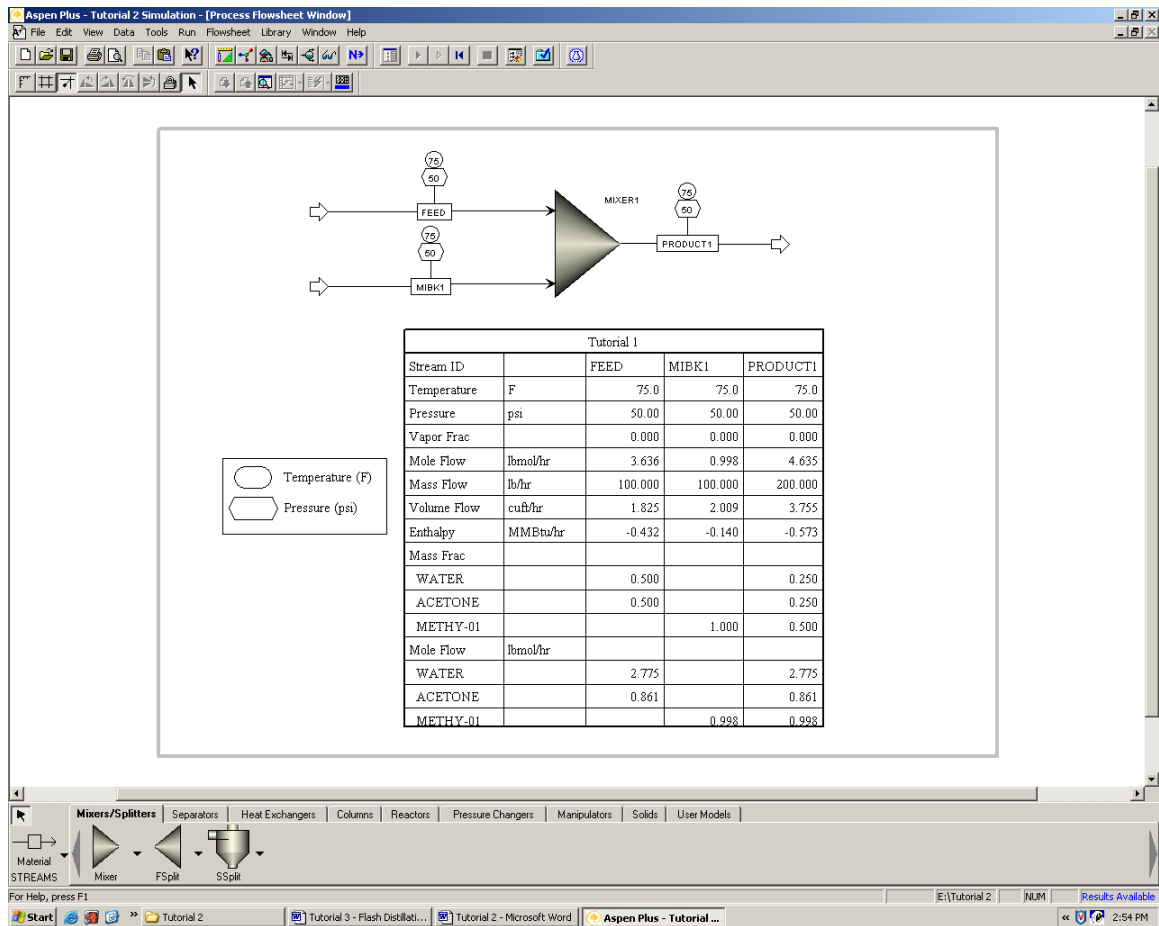
Figure 8: Page Break Preview

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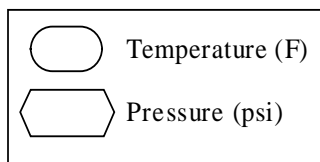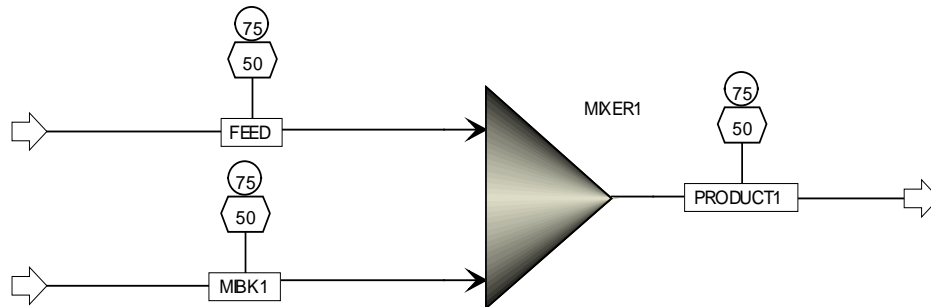
Tutorial 1				
Stream ID		FEED	MIBK1	PRODUCT1
Temperature	F	75.0	75.0	75.0
Pressure	psi	50.00	50.00	50.00
Vapor Frac		0.000	0.000	0.000
Mole Flow	lbmol/hr	3.636	0.998	4.635
Mass Flow	lb/hr	100.000	100.000	200.000
Volume Flow	cuft/hr	1.825	2.009	3.755
Enthalpy	MMBtu/hr	-0.432	-0.140	-0.573
Mass Frac	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

Temperature (F)

Pressure (psi)

```
;
;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.

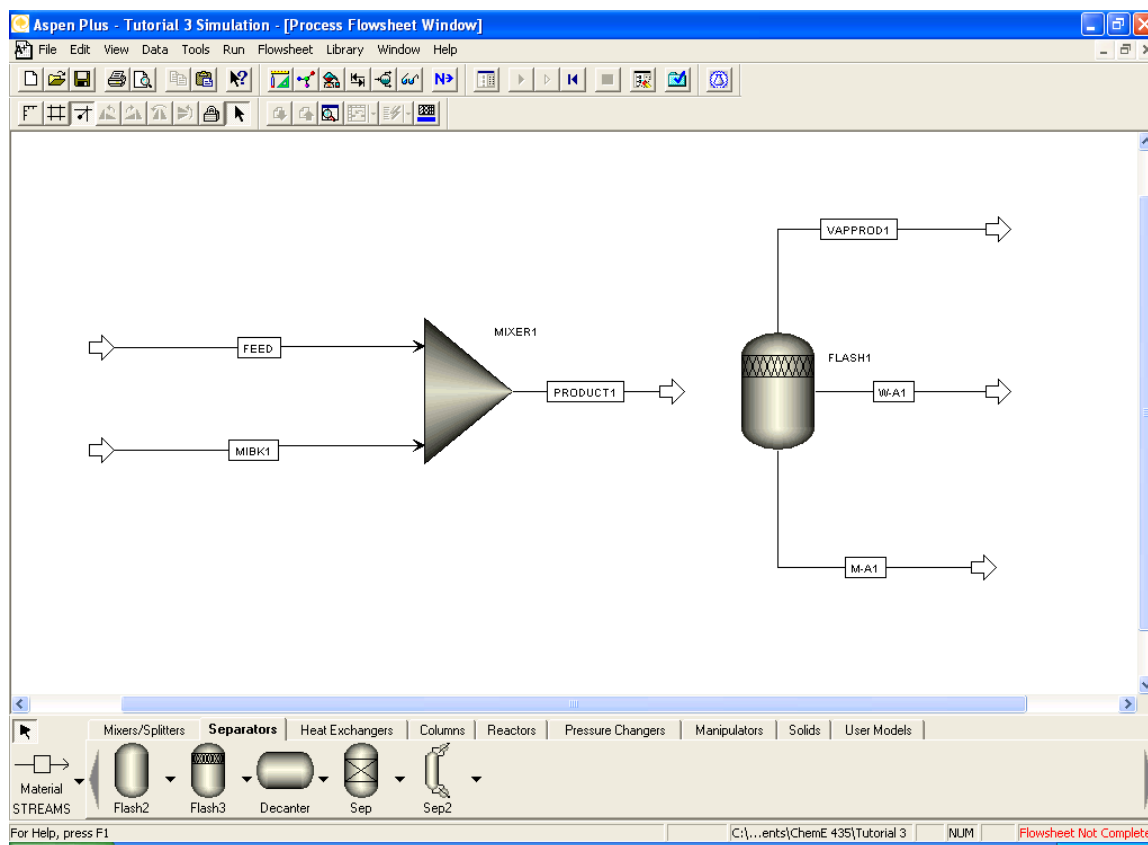Aspen Tutorial #3

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.

Aspen Tutorial #3
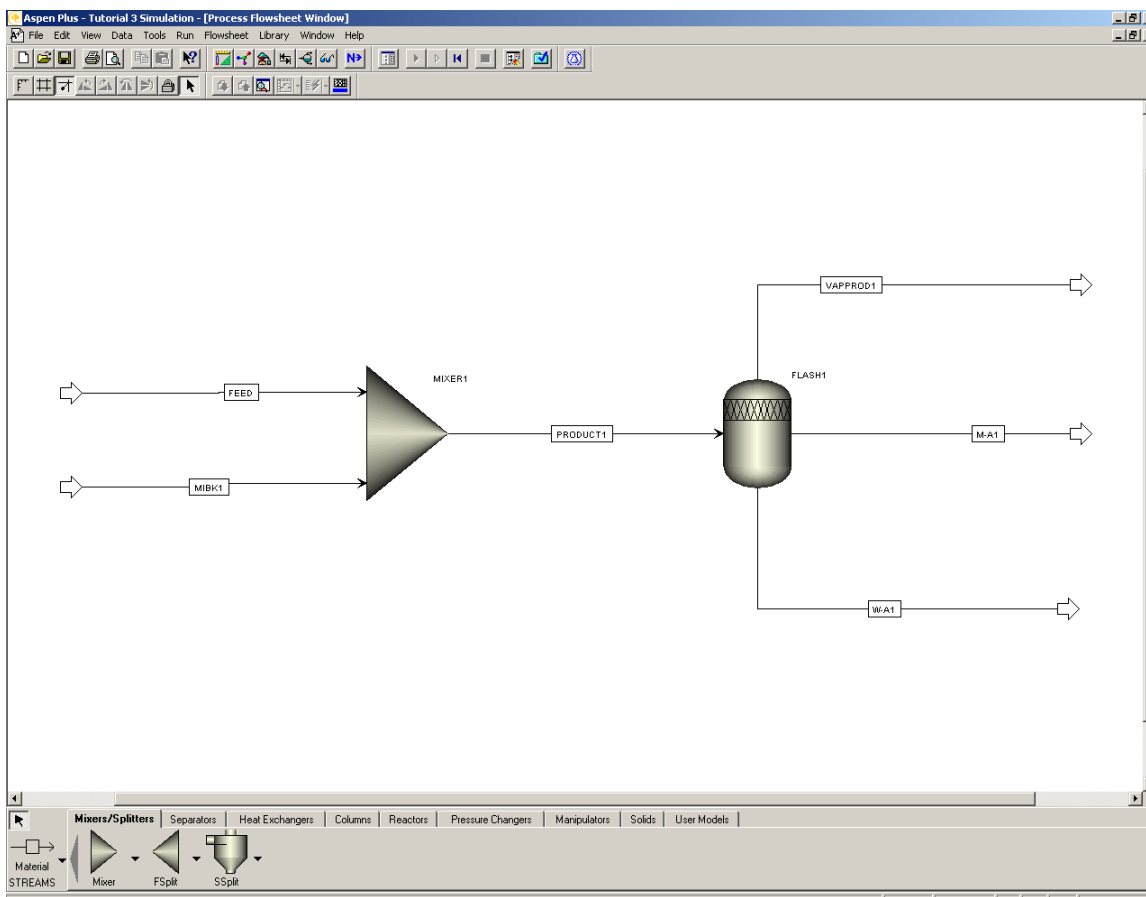
Figure 2: Completed Flowsheet

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.
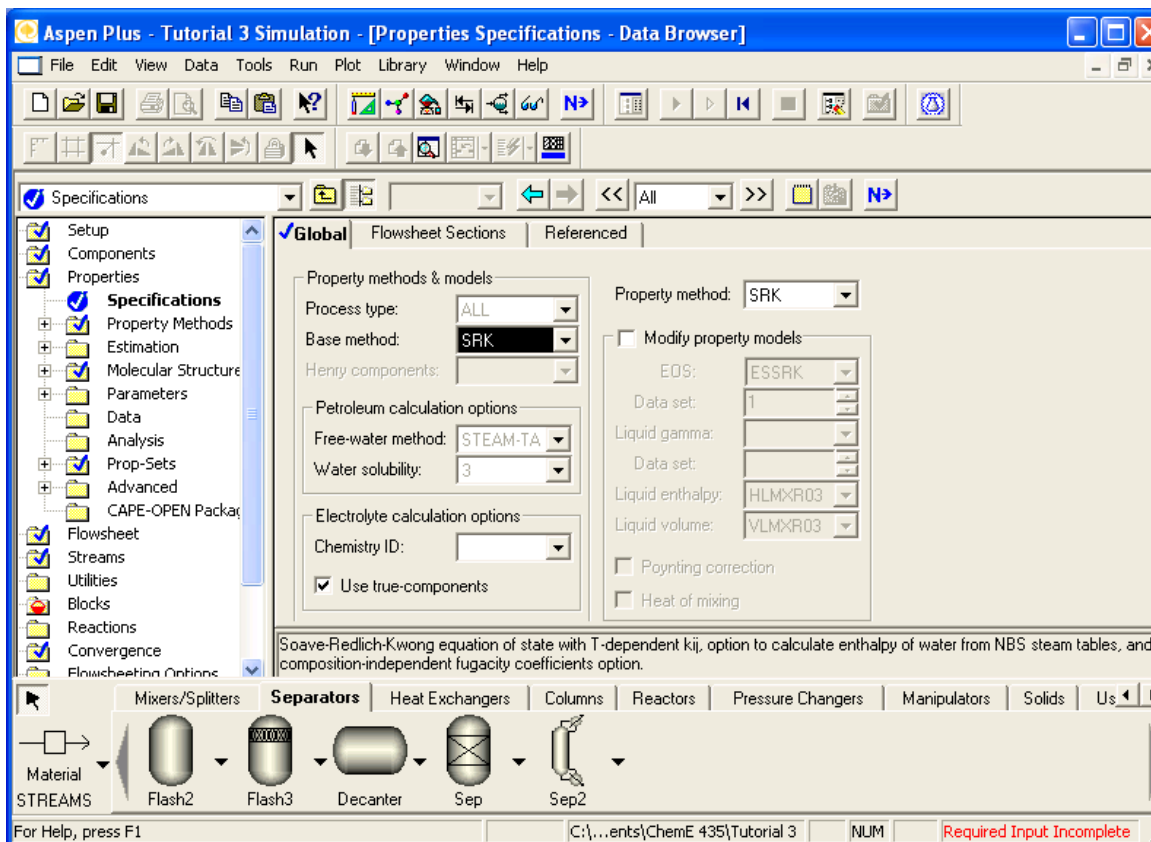
Figure 3: Thermodynamic Base Method

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 (75° F and 50 psi). After inputting these two values you will notice that the Simulation Status changes to "Required Input Complete".
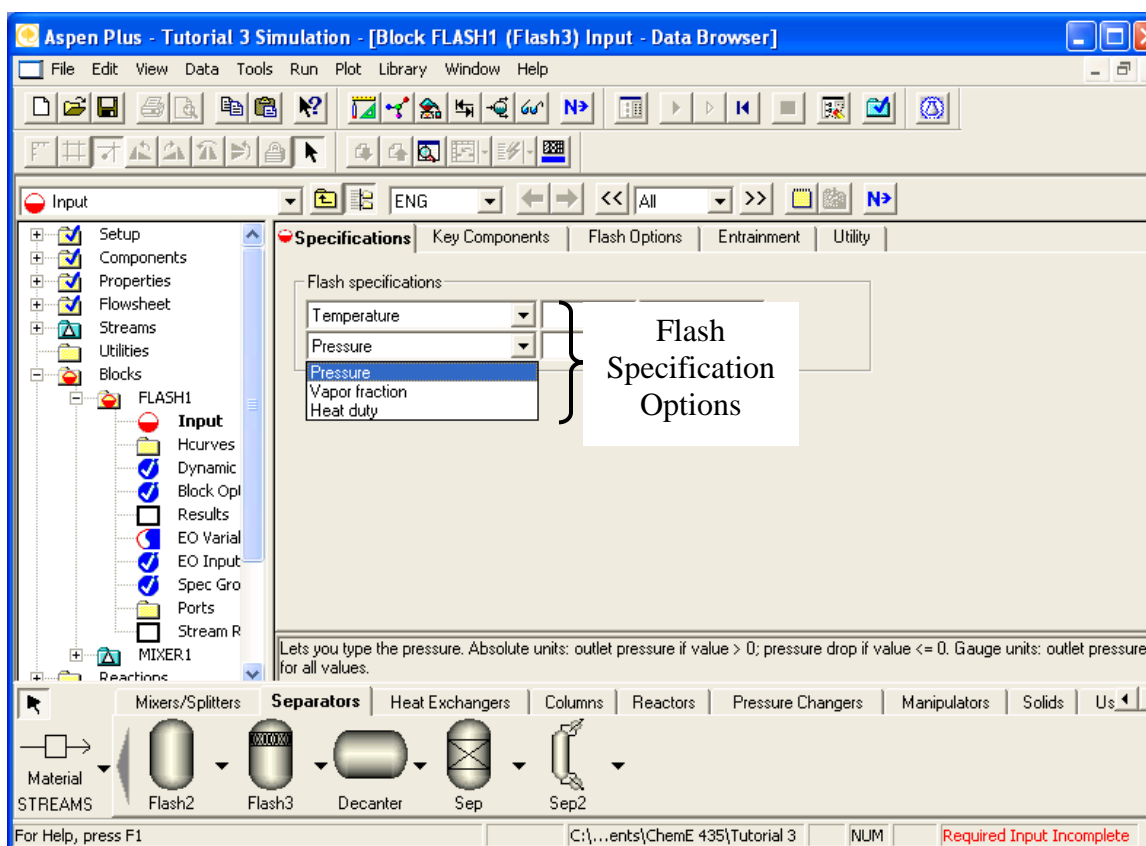
Figure 4: Flash Data Input Options

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).

Aspen Tutorial #3
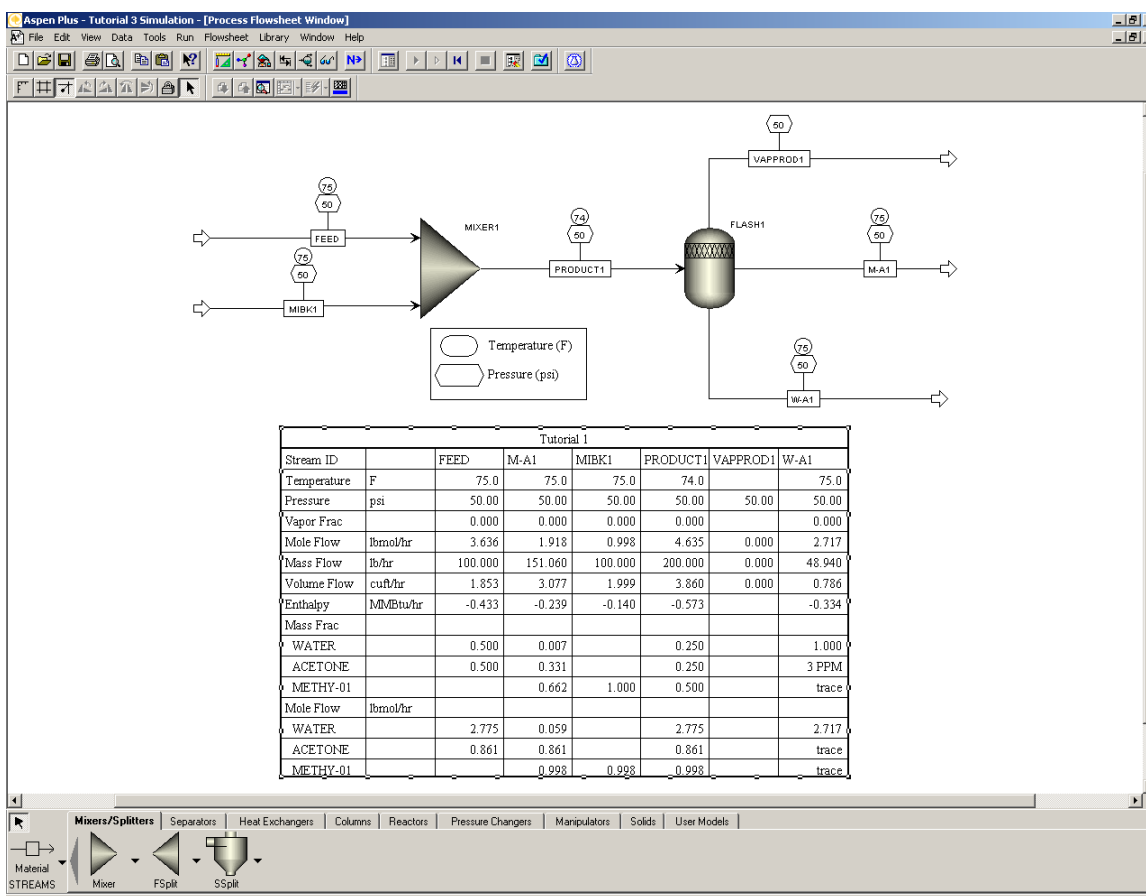
Figure 5: Completed Process Flowsheet

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.

Aspen Tutorial #3
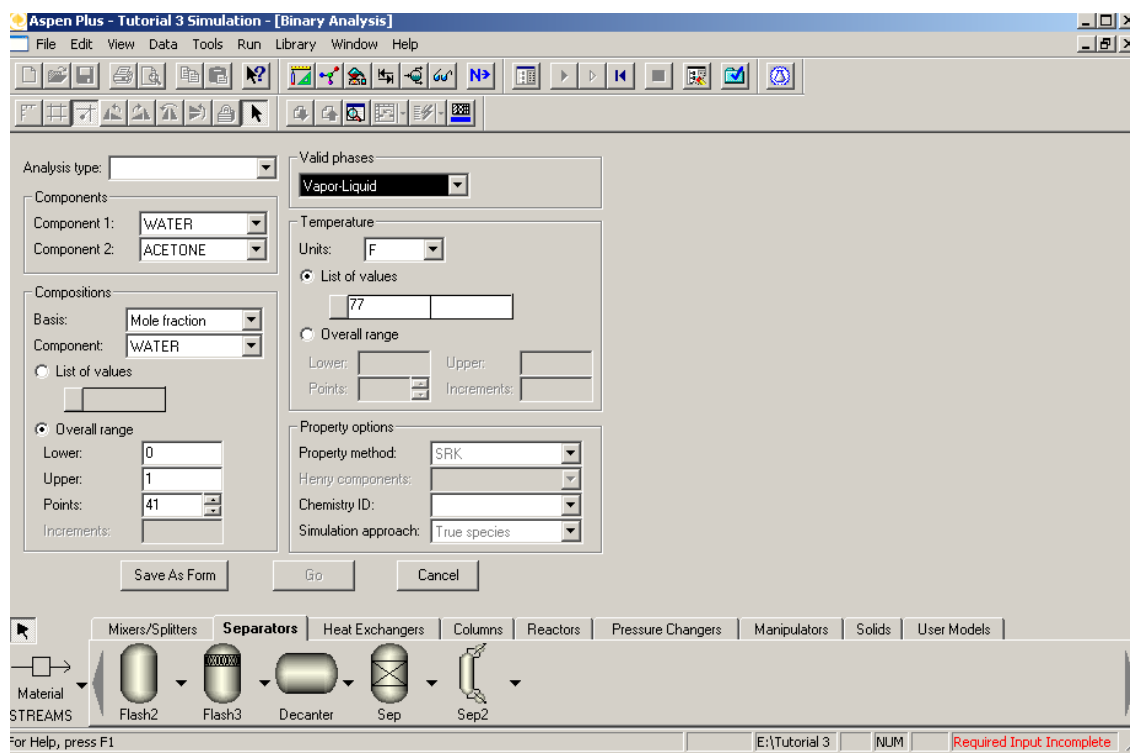
Figure 6: Binary Analysis Window

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).

Aspen Tutorial #3
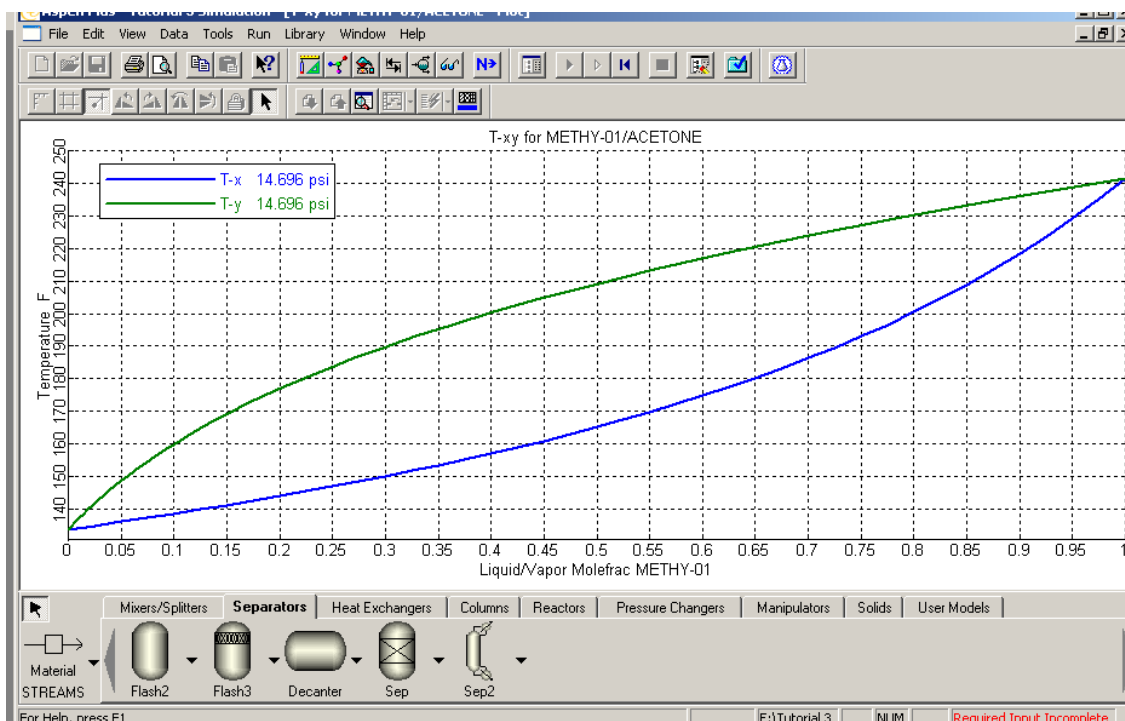
Figure 7: Txy Plot for MIBK and Acetone

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.

Aspen Tutorial #3
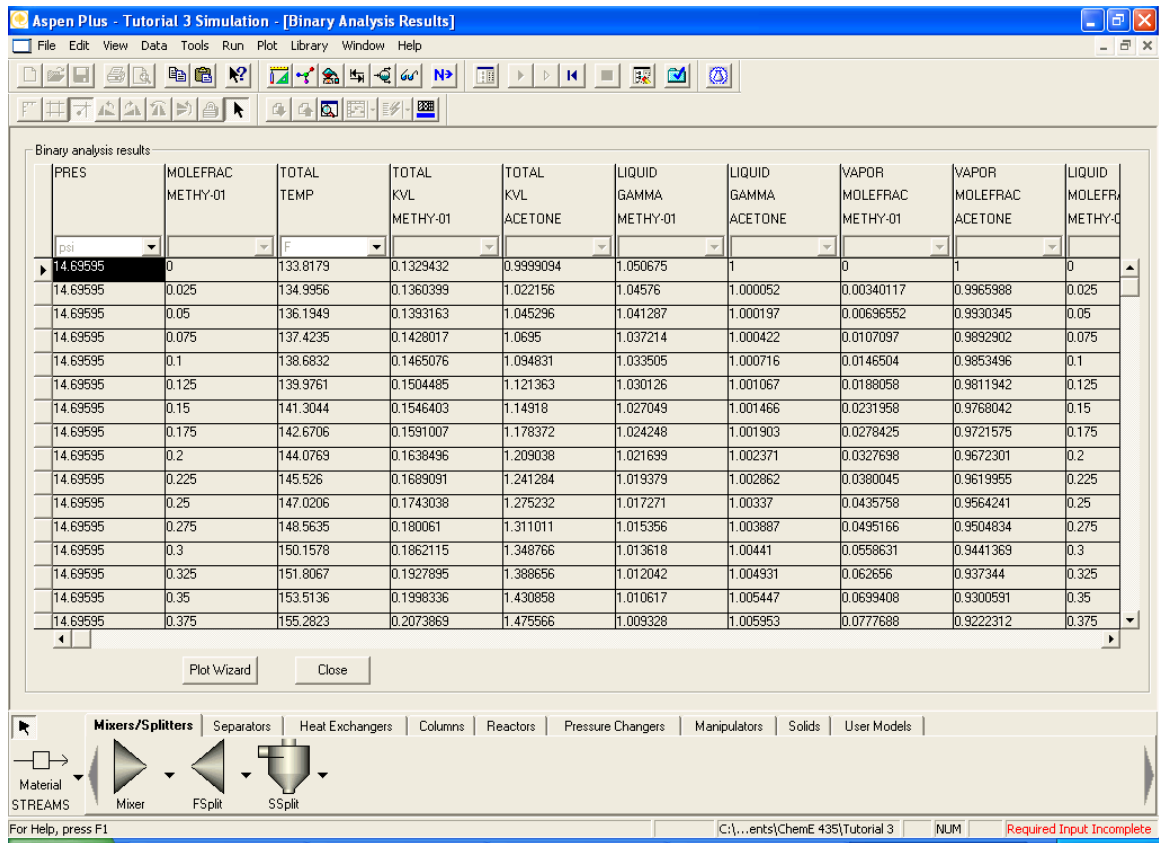
Figure 8: Binary Analysis Results Window

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:

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

Aspen Tutorial #3
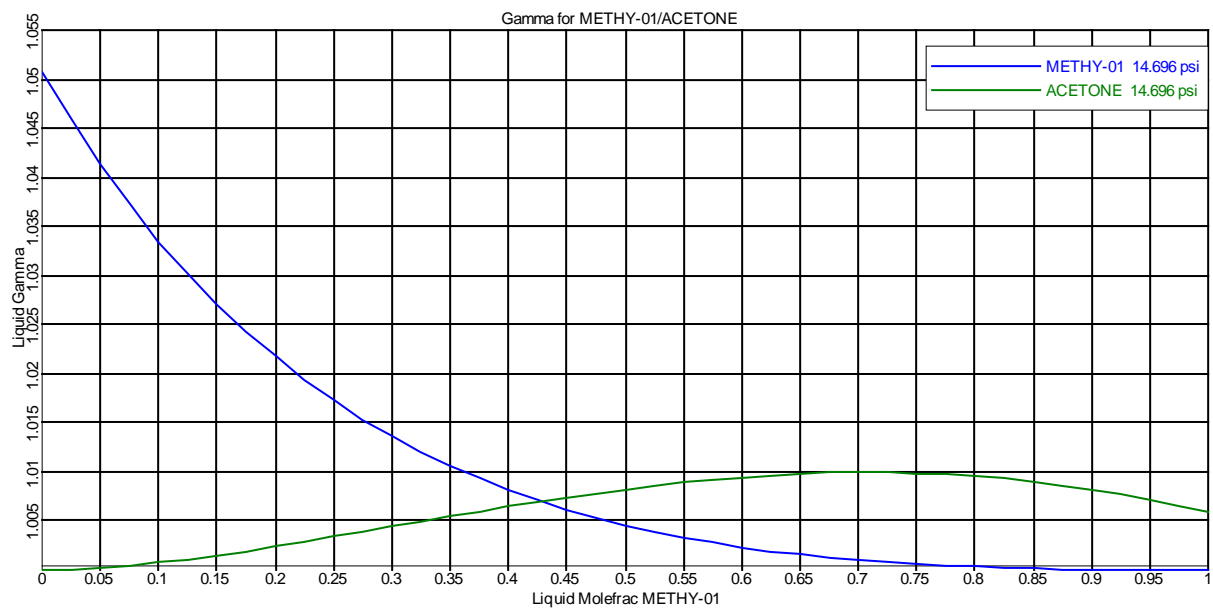
Aspen Tutorial #4: Thermodynamic Methods

Outline:

- Problem Description
- Available Thermodynamic Property Methods
- Recommended Methods for Selected Applications
- Influence of Thermodynamic Method on Our Problem

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.

In our previous tutorials, I have been telling you which thermodynamic methods to choose based on that week's update to the simulation. This week we will be covering the many thermodynamic methods that are available in Aspen and examining their influence on the results of our simulation. This tutorial is a little shorter than the previous ones, but the information presented here is one of the most important concepts to understand when using simulation programs. For this reason you should make sure you understand this material well.

Available Thermodynamic Property Methods:

Aspen has four main types of Property Methods: Ideal, Equation of State, Activity Coefficient, and Special Systems. In addition, an advanced user can modify any of these available methods or create a new property method on their own.

Open up your Aspen simulation. Select the Help Topics under Help on the Menu Bar. This will open up the Aspen Plus Help window as shown in Figure 1. On the left hand side of the screen, select the Index tab and type in Property Methods. Select Property Methods in the list on the left hand side and then select the Available Property Methods option.
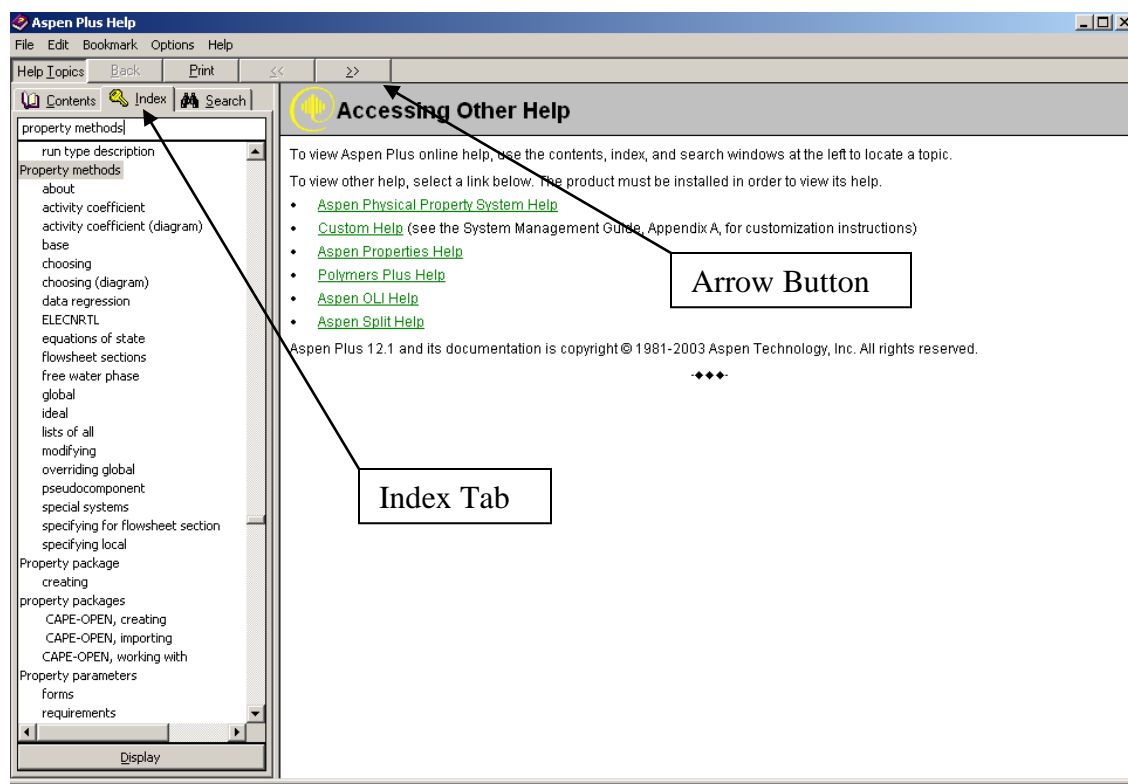
Figure 1: Aspen Plus Help

You can use the right arrow button to page through the Help window's information on the available thermodynamic methods. Hitting it once will bring you to the first group of available methods, which is the Ideal group, as shown in Figure 2. Thermodynamic phase equilibrium can be determined in a number of ways, including chemical potential, fugacity, activities, activity coefficients, or the equilibrium distribution ratio. You will notice that the Ideal methods rely on using ideal system equations to calculate the equilibrium distribution ratio (K), which is then used to determine the equilibrium conditions.
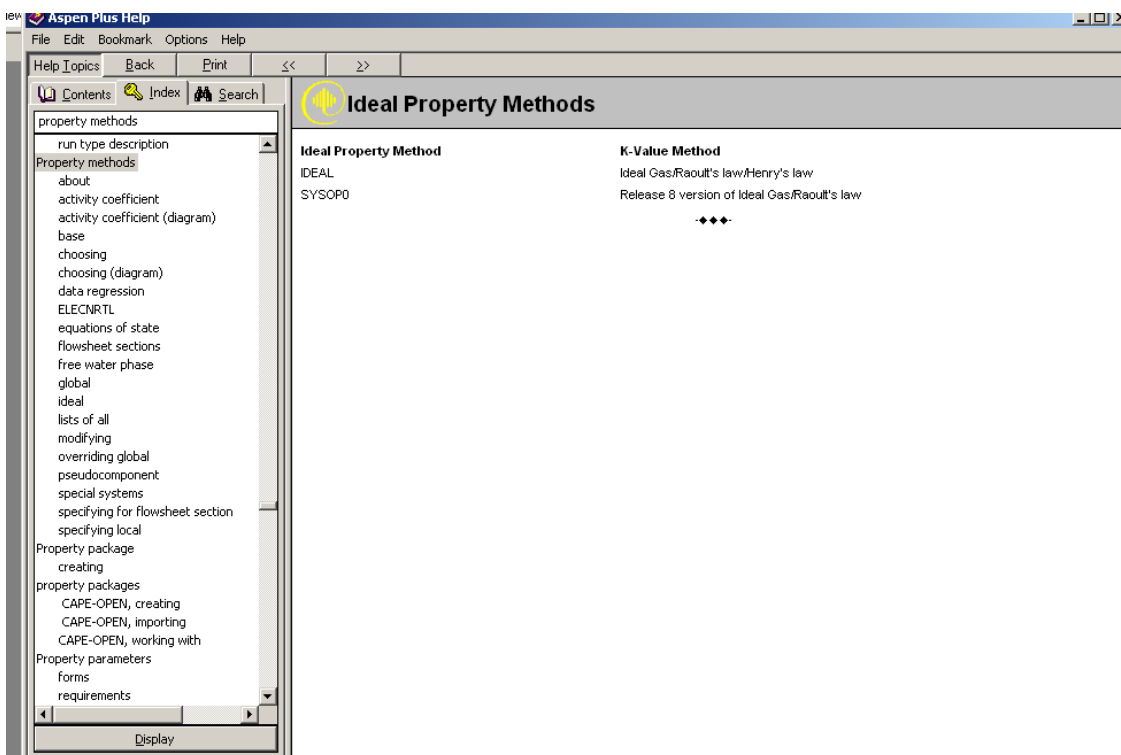
Figure 2: Ideal Property Methods

If you hit the arrow again, the window will move on to the Equation of State Property Methods. These methods use the various equations of state that are learned about in chemical engineering thermodynamics, to calculate the equilibrium distribution ratio. The two most familiar methods from this section are listed in the table below. You will also notice that Aspen provides many of the minor variations to the most common methods (i.e. PRMHV2 – a modified Peng-Robinson equation).

Table 1: Most Common EOS Property Methods

EOS Property Method	K-Value Method
PENG-ROB	Peng-Robinson
RK-SOAVE (also SRK)	Redlich-Kwong-Soave

The next group of available property methods is the Activity Coefficient group. This group uses various relationships to calculate the liquid phase activity coefficient and then calculate the vapor fugacity using a second relationship. Some of the most common methods for this group are listed in Table 2. As before, there are many modifications to the basic set of choices, which are useful for specific applications.

Table 2: Common Activity Coefficient Property Methods

Property Method	Liquid Phase Activity Coefficient	Vapor Phase Fugacity
NRTL (Non-Random Two Liquid)	NRTL	Ideal Gas
UNIFAC	UNIFAC	Redlich-Kwong
VANLAAR	Van Laar	Ideal Gas
WILSON	Wilson	Ideal Gas

Hitting the arrow button one more time will bring you to the final group of Property Methods. This is the Special Systems group. You will notice that this group provides the available methods for amine systems, solids systems, and steam systems. This is all the time we will spend here, since our system is not one of these special cases.

Recommended Methods for Potential Applications:

Selecting the arrow button one more time will bring you to the Choosing a Property Method help screen. The Aspen Plus Help provides two different methods to suggest the appropriate property methods. The first of these is a listing of the appropriate methods for certain industries and the second is a diagram that a user can step through to choose an appropriate method.

In this tutorial we will go through the "Recommended property methods for different applications" option. Select that choice in the help window. This will open up the window shown in Figure 3.

Use the arrow button to walk through the various applications that are presented here. You will notice that each application is further broken down by the specific operations in that industry. Most of these operations have two or three suggested thermodynamic methods. Stop on the Chemicals application screen as this is the industrial application that is most like our particular simulation. Take note of which thermodynamic methods most often appear for these applications. We will be testing out a few of them in our simulation, in the final portion of this tutorial.
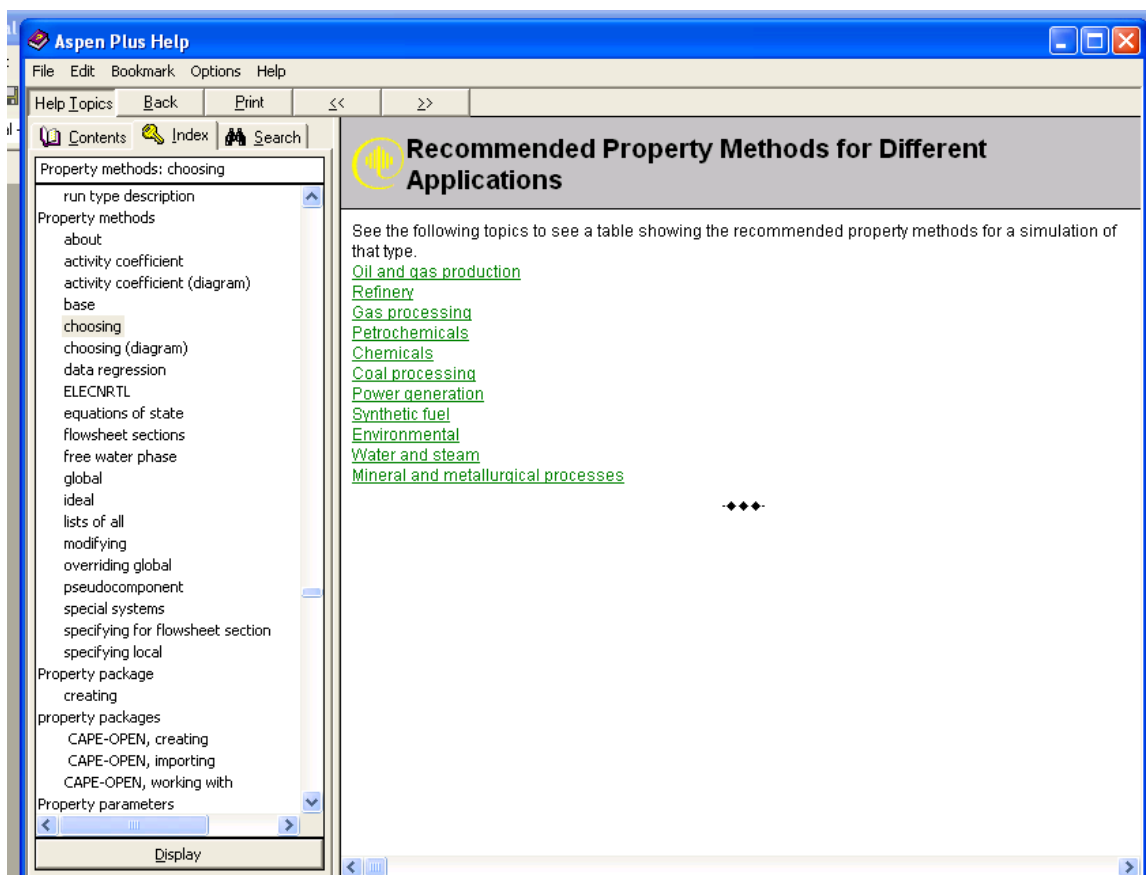
Figure 3: Recommended Property Methods for Different Applications

Continue to walk through the other application screens until you have looked at all of them and then close the help window.

Influence of Thermodynamic Method on Our Problem:

The last time we ran our simulation we used the SRK thermodynamic method. For our homework this week, we will be comparing the simulation results obtained with this method to those obtained through three other methods, IDEAL, WILSON, and NRTL.

Using what you have learned from the other Tutorials, rerun your simulation with each of the three thermodynamic methods listed above. Don't forget to reinitialize your simulation between runs. When you run the case with the WILSON and NRTL thermodynamic methods, you will be required to go into the Properties tab in the Data Browser. However, you only need to open up the window Wilson-1 or NRTL-1 under Binary Parameters to allow the default parameters to be recognized as input. You do not need to change any of the values shown in these screens.

For the homework assignment, a stream table from each run and a sentence or two highlighting the differences will suffice.

Next week: Sensitivity Analysis and Transport Properties

Tutorial #4 Homework and Solution

Question:

Compare the simulation results from last week to those obtained with the following three thermodynamic methods: IDEAL, WILSON, and NRTL. Show the stream table results for each thermodynamic method and write a sentence or two summarizing your findings.

Solution:

SRK Results (last week):

Tutorial 4							
Stream ID		FEED	M-A1	MIBK1	PRODUCT	VAPPROD	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

IDEAL Results:

Tutorial 4							
Stream ID		FEED	M-A1	MIBK1	PRODUCT	VAPPROD	W-A1
Temperature	F	75.0	75.0	75.0	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		
Mole Flow	lbmol/hr	3.636	4.635	0.998	4.635	0.000	0.000
Mass Flow	lb/hr	100.000	200.000	100.000	200.000	0.000	0.000
Volume Flow	cuft/hr	1.825	3.755	2.009	3.755	0.000	0.000
Enthalpy	MMBtu/hr	-0.432	-0.573	-0.140	-0.573		
Mass Frac							
WATER		0.500	0.250		0.250		
ACETONE		0.500	0.250		0.250		
METHY-01			0.500	1.000	0.500		
Mole Flow	lbmol/hr						
WATER		2.775	2.775		2.775		
ACETONE		0.861	0.861		0.861		
METHY-01			0.998	0.998	0.998		

Aspen Tutorial #4

WILSON Results:

Tutorial 4							
Stream ID		FEED	M-A1	MIBK1	PRODUCT	VAPPROD	W-A1
Temperature	F	75.0	75.0	75.0	84.9		
Pressure	psi	50.00	50.00	50.00	50.00	50.00	50.00
Vapor Frac		0.000	0.000	0.000	0.000		
Mole Flow	lbmol/hr	3.636	4.635	0.998	4.635	0.000	0.000
Mass Flow	lb/hr	100.000	200.000	100.000	200.000	0.000	0.000
Volume Flow	cuft/hr	1.825	3.755	2.009	3.781	0.000	0.000
Enthalpy	MMBtu/hr	-0.436	-0.579	-0.140	-0.577		
Mass Frac							
WATER		0.500	0.250		0.250		
ACETONE		0.500	0.250		0.250		
METHY-01			0.500	1.000	0.500		
Mole Flow	lbmol/hr						
WATER		2.775	2.775		2.775		
ACETONE		0.861	0.861		0.861		
METHY-01			0.998	0.998	0.998		

NRTL Results:

Tutorial 4							
Stream ID		FEED	M-A1	MIBK1	PRODUCT	VAPPROD	W-A1
Temperature	F	75.0	75.0	75.0	65.3		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	1.938	0.998	4.635	0.000	2.696
Mass Flow	lb/hr	100.000	141.052	100.000	200.000	0.000	58.948
Volume Flow	cuft/hr	1.825	2.772	2.009	3.729	0.000	1.011
Enthalpy	MMBtu/hr	-0.435	-0.246	-0.140	-0.576		-0.329
Mass Frac							
WATER		0.500	0.041		0.250		0.751
ACETONE		0.500	0.263		0.250		0.220
METHY-01			0.697	1.000	0.500		0.030
Mole Flow	lbmol/hr						
WATER		2.775	0.319		2.775		2.456
ACETONE		0.861	0.638		0.861		0.223
METHY-01			0.981	0.998	0.998		0.017

You will notice in the stream tables above that both the IDEAL and WILSON thermodynamic methods do not predict any separation of our two liquid streams in the Flash separator (indicated by the zero flow in stream W-A1). However, the NRTL thermodynamic method predicts a separation that is less efficient than that predicted by the SRK method from last week. You will remember that in Tutorial #3 I mentioned that the results with the SRK thermodynamics were better than what really occurs and this is supported by these results.

Aspen Tutorial #5: Sensitivity Analysis and Transport Properties

Outline:

- Problem Description
- Updating the Simulation
- Sensitivity Analysis
- Transport Properties

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.

Up to this point we have not maximized our use of Aspen's computational abilities. Often times in chemical engineering we are faced with problems that have iterative solutions or iterative steps on the way to a desired result (i.e. purity of a component in a separation process based on a feed of another). This week we will be using Aspen to calculate the flow rate of a second feed stream of MIBK, in order to get the desired >90% purity of our water stream through the use of a sensitivity analysis. During a sensitivity analysis (or design specification) Aspen iterates its calculation sequence through a range of values provided for an independent variable, in order to obtain a specified result for a dependent variable (within a certain tolerance).

Updating the Simulation:

The most realistic separation results that we obtained last week were based on using the NRTL thermodynamic method. Make sure your simulation is set to this base method and then reinitialize your simulation.

Add a second mixer and a second flash separation unit to your process flowsheet and name them as you see fit. Connect the stream that is primarily water and acetone (the stream off of the bottom of the first flash separator) to the new mixer and add in a new feed stream of MIBK that also feeds into this new mixer. Next, connect the product from this mixer to the new flash separation unit and add in the required product streams. Your process flowsheet should now look like that seen in Figure 1.
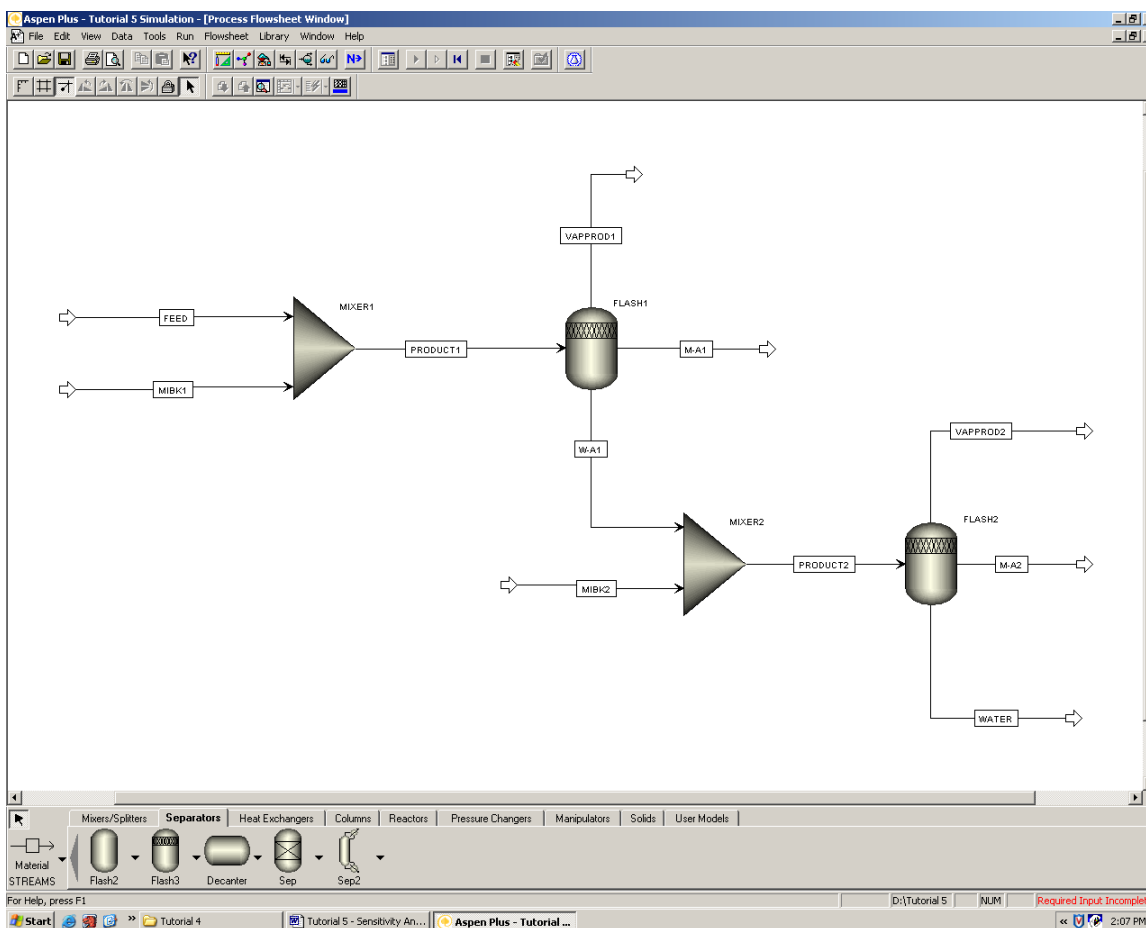
Aspen Tutorial #5

Figure 1: Updated Process Flowsheet

Now open up the Data Browser window to update the inputs for the new additions to your process flowsheet. The new feed stream of MIBK should have a flow rate of 50 lbs/hr of pure MIBK at a temperature of 75° F and a pressure of 50 psi. The new mixer and flash separation units should be specified to be at 75° F and 50 psi.

If you run the simulation at this point, you should get results similar to those seen in the stream table shown in Figure 2. You will notice that we do not get the desired 90% purity of the water stream that is specified in the original problem description. While we could simply rerun the simulation a few times to determine a feed rate of MIBK that would give us this desired purity, we will instead program Aspen to complete the iterations for us before reporting the results.

You may notice that the stream table shown in Figure 2 does not include all of the streams. You might remember that this was discussed in Tutorial #2 under the Display Options. I have shown only the important feed and product streams to save space (I have eliminated all of the intermediate streams and the product streams with no flow).

40

Tutorial 5 - Sensitivity Analysis							
Stream ID		FEED	MIBK1	MIBK2	M-A1	M-A2	WATER
Temperature	F	75.0	75.0	75.0	75.0	75.0	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	0.000
Mole Flow	lbmol/hr	3.636	0.998	0.499	1.938	0.725	2.470
Mass Flow	lb/hr	100.000	100.000	50.000	141.052	59.825	49.123
Volume Flow	cuft/hr	1.825	2.009	1.004	2.772	1.181	0.818
Enthalpy	MMBtu/hr	-0.435	-0.140	-0.070	-0.246	-0.096	-0.303
Mass Frac							
WATER		0.500			0.041	0.027	0.868
ACETONE		0.500			0.263	0.127	0.108
METHY-01			1.000	1.000	0.697	0.846	0.023
Mole Flow	lbmol/hr						
WATER		2.775			0.319	0.089	2.367
ACETONE		0.861			0.638	0.131	0.092
METHY-01			0.998	0.499	0.981	0.505	0.012

Figure 2: Stream Results with 50 lbs/hr MIBK Feed

Sensitivity Analysis:

Select the Flowsheeting Options tab in the Data Browser window and open up the Design Spec option. At the bottom of the screen, select the new button and choose a name for this design specification. When you have done this the Data Browser window should look like that seen in Figure 3. You will notice that there are three areas where we must input data in order for the required input to be complete. These are the tabs Define, Spec, and Vary.

In the Define tab the user must set the dependent variable that they are interested in. For our case, this is the purity of the water product stream (or mass fraction of water). Select new at the bottom of this screen and name the new variable WATER. After hitting OK, the Variable Definition window will appear. In this window we need to specify that we want our variable to be the mass fraction of water in the "pure" water product stream. In the type box, select MASS-FRAC (you may want to note the many types of design specifications one can specify by scrolling through the options in the type box at this time). In the stream box that then appears, select your water product stream and under the component box, select WATER. At this point your Variable Definition window should look similar to that seen in Figure 4. The only difference should be in the stream name, unless you have used the same stream names I have in your process flowsheet. Hit the close button when you have completed this.
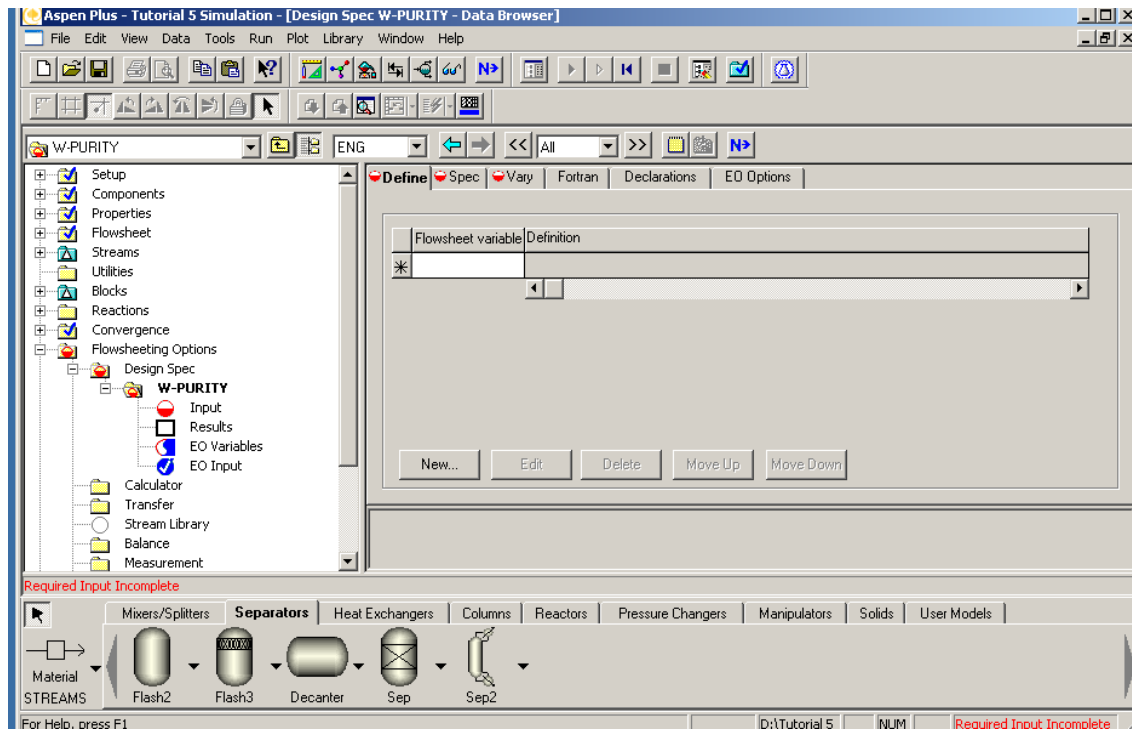
Aspen Tutorial #5

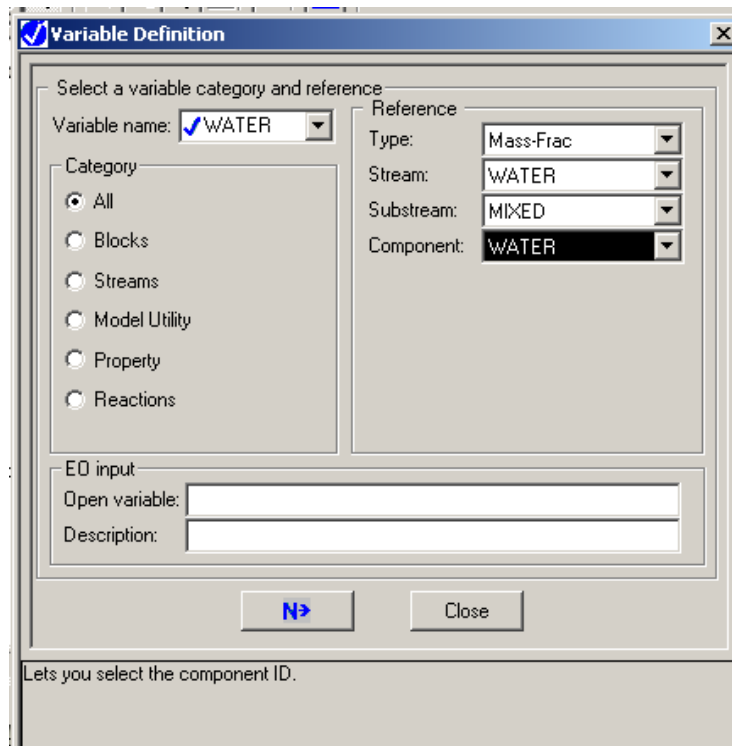**Figure 3: Design Specification Window**

Figure 4: Completed Variable Definition Window

For our purposes we are now done inputting information into the Define tab and can move on to the Spec tab. You will notice that we have three values we must input into

this window. The first, Spec, is the dependent variable that we want to set a target value for. This is the variable that we just defined in the Define tab as WATER. Type this into this box. Target is the numeric value that we would like our dependent variable to be equal to at the completion of the calculation iterations. Our target value is 90%, or 0.90. Finally, Tolerance is how close the solution determined by Aspen must be to our target value before it is deemed acceptable. For our purposes, a tolerance of 0.1% is acceptable (this is input as 0.001). After inputting this, the Spec window should look like that seen in Figure 5.
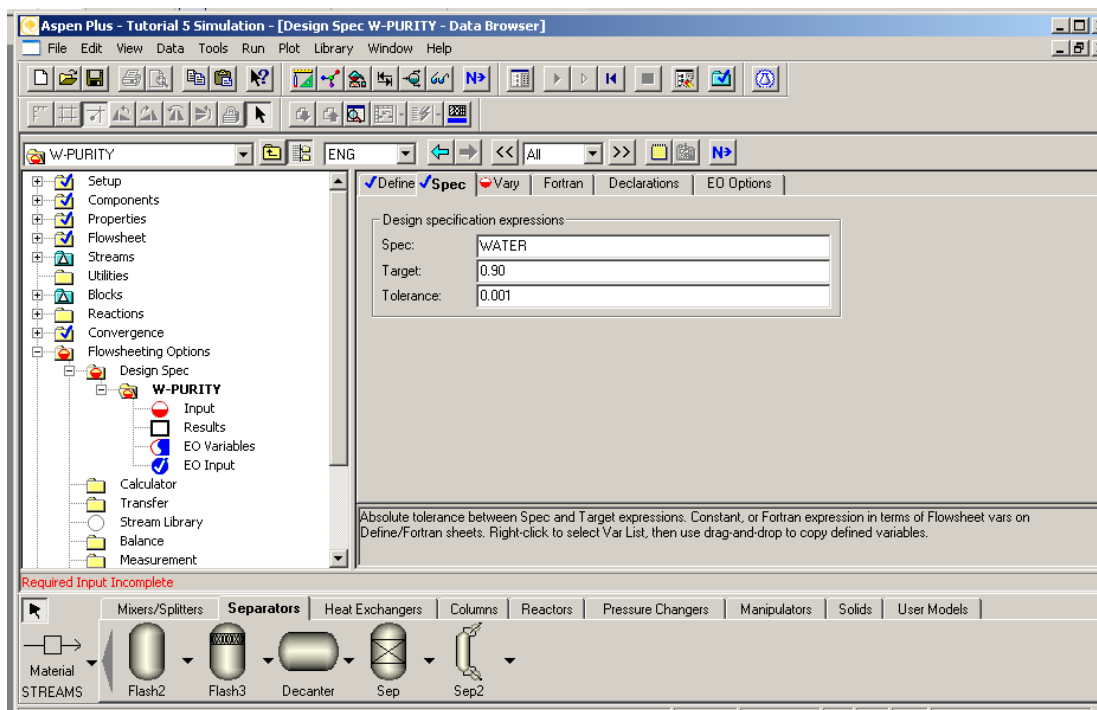

Figure 5: Completed Spec Window

To complete the input for our sensitivity analysis, we must input which variable is to be varied. This is done under the Vary tab. In this simulation, we are varying the flow rate of MIBK in the second feed stream of MIBK (mine is entitled MIBK2). This is the stream we just added to our simulation. Under the Vary tab select MASS-FLOW under the type tab. Again, it is worth pointing out the many different variables that can be manipulated in Aspen. Under stream, select the stream that corresponds to your second feed stream of MIBK. Next, select METHY-01 from the components list. At this point the Vary tab should look like that seen in Figure 6.

The values placed into the Manipulated Variable Limits boxes indicate the range that Aspen can use during its iteration calculations. One thing to note is that the original input value under the stream inputs must fall within the range that is input here. Remember our original input was 50 lbs/hr. For this tutorial, input a variable range from 25-100 lbs/hr. The other blocks that can be filled on this screen relate to the step size that Aspen takes during its iteration calculations. It is not necessary for the user to input values into these blocks, and we will use the default Aspen values.
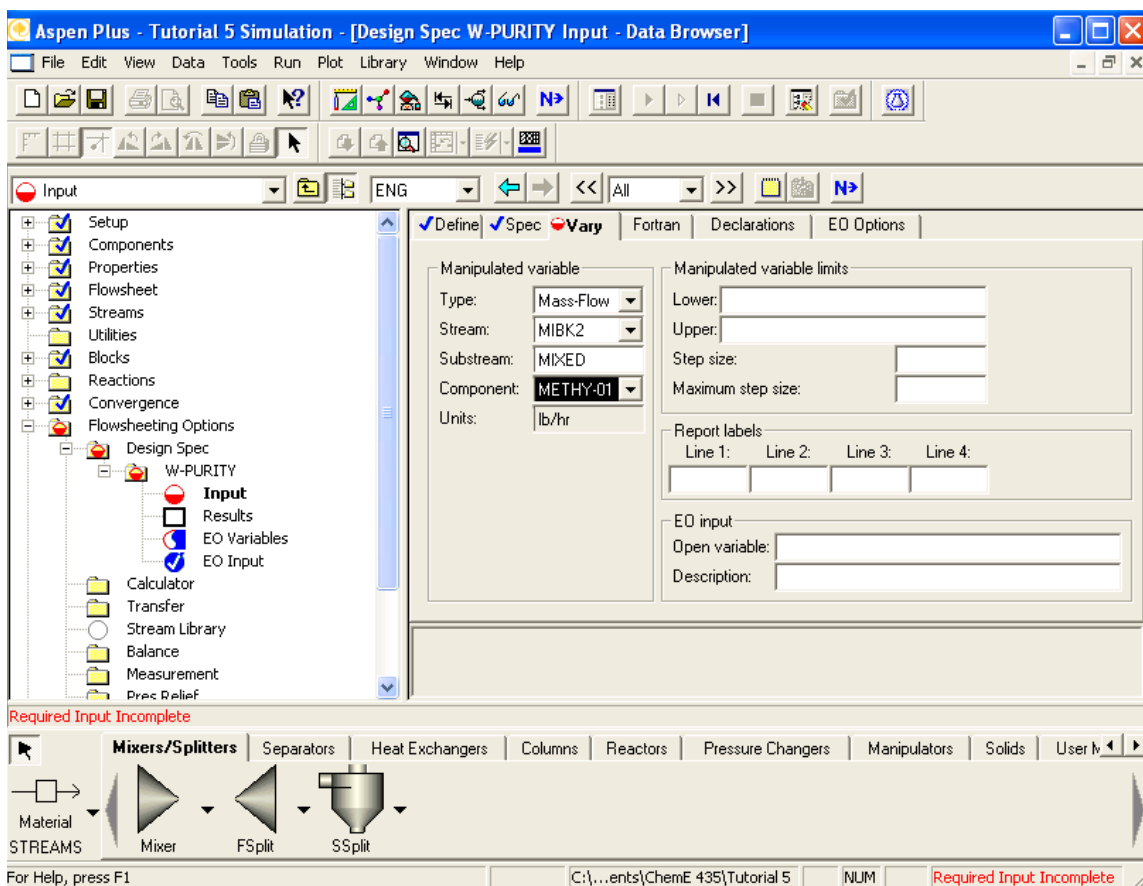
Figure 6: Vary Tab Options

At this point, our required input should again be complete. The completed Vary tab is shown below in Figure 7. We are now ready to run the simulation again and check its convergence based on our input design specifications. Hit the run button at this time and when the computer has finished its calculations, open up the Run Control Panel (see Tutorial #2 for help with this).

The Run Control Panel indicates how many iterations Aspen made during its determination of the flow rate that met our design specification. If completed correctly, your simulation should have no warnings and no errors indicated in this window. You will notice in Figure 8 that my simulation took 5 iterations to determine results that were within the specified tolerance. We must also complete a cursory check of the simulation results as discussed in Tutorial #2. This is especially important now that we have introduced design specifications into the simulation. Close the Run Control Panel window and open up the data browser to confirm that the simulation converged with reasonable results.

Aspen Tutorial #5
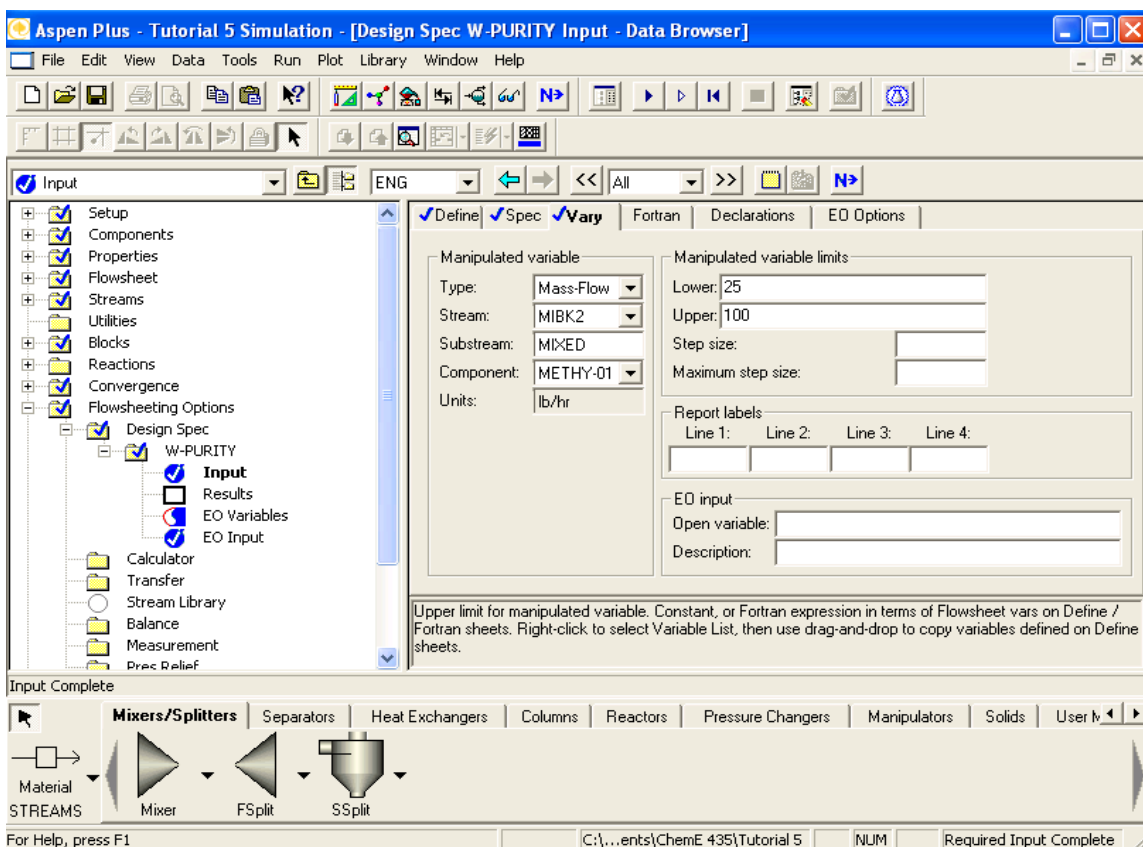
Figure 7: Completed Vary Window

You will notice that the Convergence option under the Results Summary Tab in the Data Browser window now has results. This window indicates the final value of the variable and the error associated with this variable as shown in Figure 9. The Error column indicates how far off the final dependent variable was from the specified value and the Error / Tolerance column indicates how closely the design specification converged. A value of 1 in this column means that the simulation barely converged while a value near 0 indicates excellent convergence.

The final place where the user can get information regarding the convergence of a simulation is under the Convergence tab in the Data Browser window. In this window one can actually see each of the values attempted by Aspen during its iteration cycle.

Aspen Tutorial #5

Figure 8: Run Control Panel

Figure 9: Convergence Results

Complete a cursory check of the other simulation results as discussed in Tutorial #2 and if all of them look acceptable, proceed on to the next section.

Transport Properties:

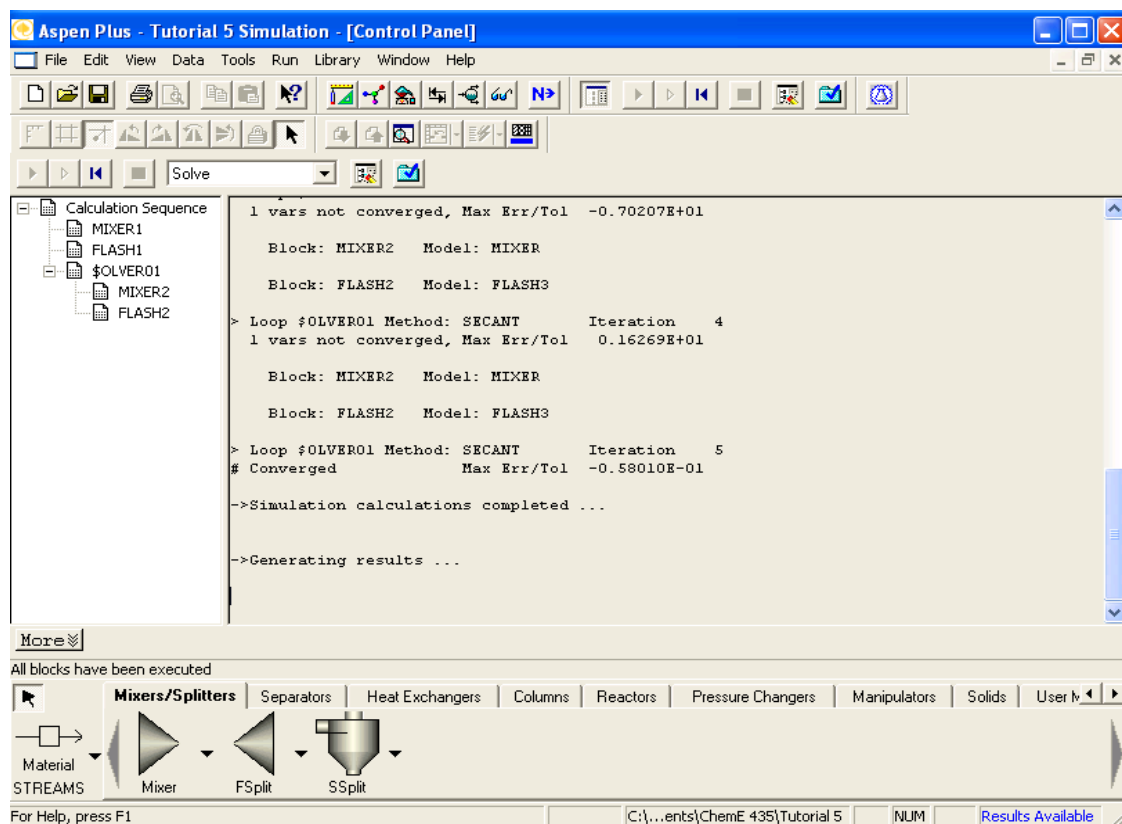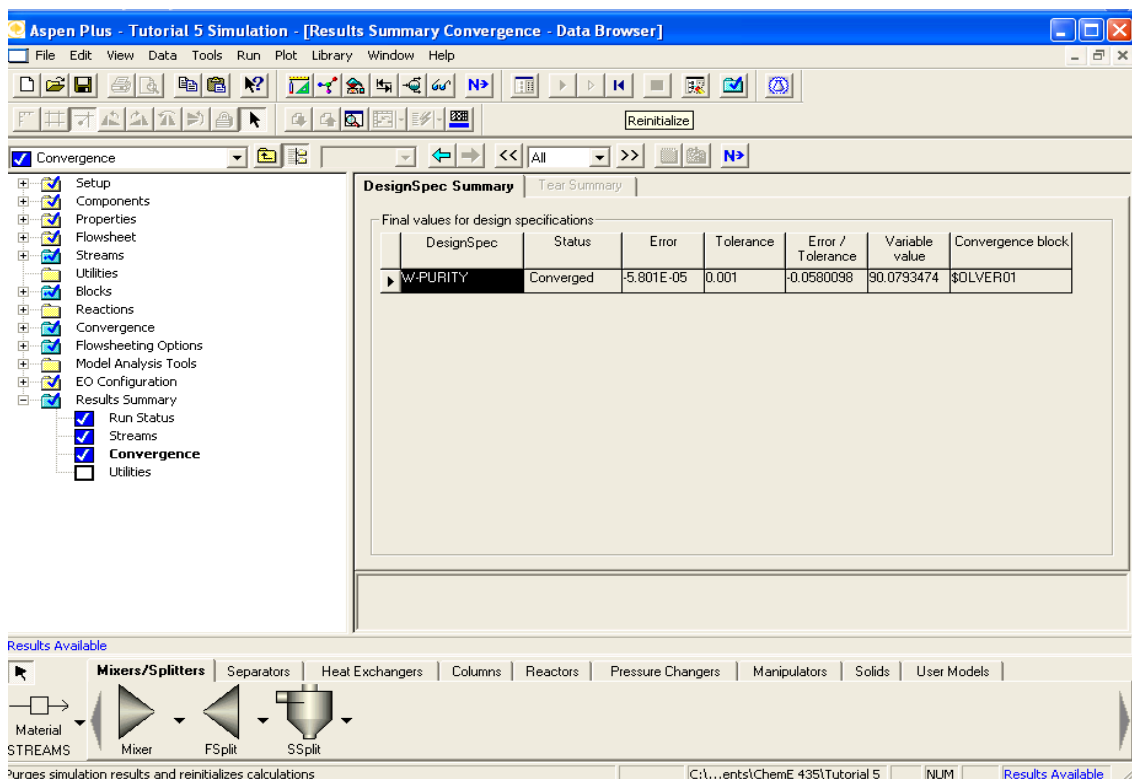Although we touched on some of the options for including selected physical properties in stream tables, we did not touch on adding those properties that are important for mass transfer (i.e. diffusivities). However, diffusivity is not one of the default variables that are reported by Aspen and it is only reported if the user defines a specific property set. The easiest way to do this is to modify an existing property set that reports other parameters of interest and then have Aspen report this property set. Open up the Prop-Sets option under the Properties tab in the Data Browser Window. Aspen has five default property sets that can easily be added to a stream table. These five are summarized in Table 1 below.

Table 1: Aspen Property Sets

Property Set	Use	Properties
HXDESIGN	Heat Exchanger Design	Thermal and Transport Properties
THERMAL	Thermal Properties	Enthalpy, Heat Capacity, Thermal Conductivity
TXPORT	Transport Properties	Density, Viscosity, Surface Tension
VLE	VL Equilibrium	Fugacity, Activity, Vapor Pressure
VLLE	VLL Equilibrium	Fugacity, Activity, Vapor Pressure

We will be modifying the TXPORT property set so that it includes diffusivity values for our system. In the Prop-Sets window, select TXPORT and hit the edit button at the bottom of the screen. The window that opens up is shown in Figure 10, on the next page.

Select the last box in the first column that is currently blank. In doing so, you will be presented with a scrolling window of physical properties that Aspen can calculate for the user. Scroll down until you find DMX, which is the variable for diffusivity in Aspen. You will notice that a description of what each physical property is appears in the bottom window as you scroll over the options. Aspen has seven built-in diffusivity models, some of which you may be familiar with. These models are summarized in Table 2.

Table 2: Diffusivity Models

Model Equation	Application
Chapman-Enskog-Wilke-Lee (Binary)	Low Pressure Vapor
Chapman-Enskog-Wilke-Lee (Mixture)	Low Pressure Vapor
Dawson-Khoury-Kobayashi (Binary)	Vapor
Dawson-Khoury-Kobayashi (Mixture)	Vapor
Nernst-Hartley	Electrolyte
Wilke-Chang (Binary)	Liquid
Wilke-Change (Mixture)	Liquid

Aspen Tutorial #5
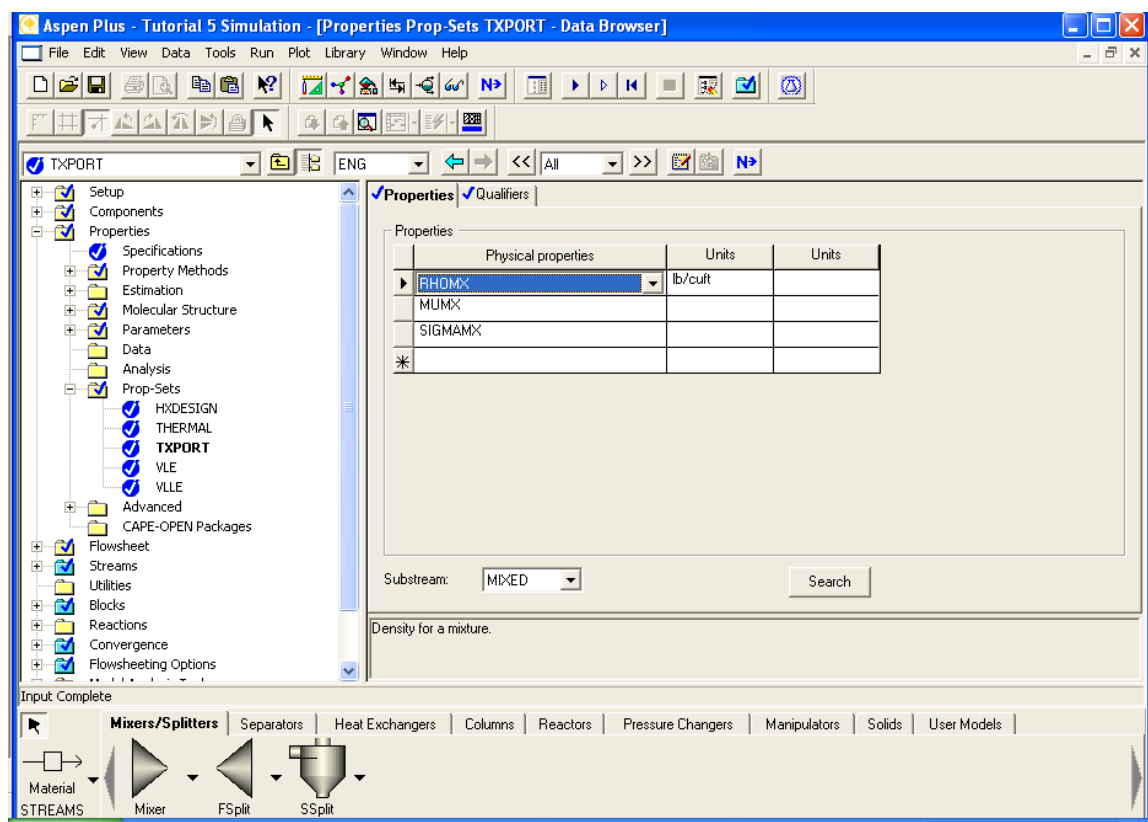
Figure 10: TXPORT Edit Window

Now select the Qualifiers tab. This window allows the user to input what phases they would like the property set to be reported for. Because we are not concerned about the vapor phase at this point, we will remove it from the reported results. Select the box marked Vapor and hit the Delete key on the keyboard. The Qualifiers tab should now look like that seen in Figure 11.

Aspen Tutorial #5
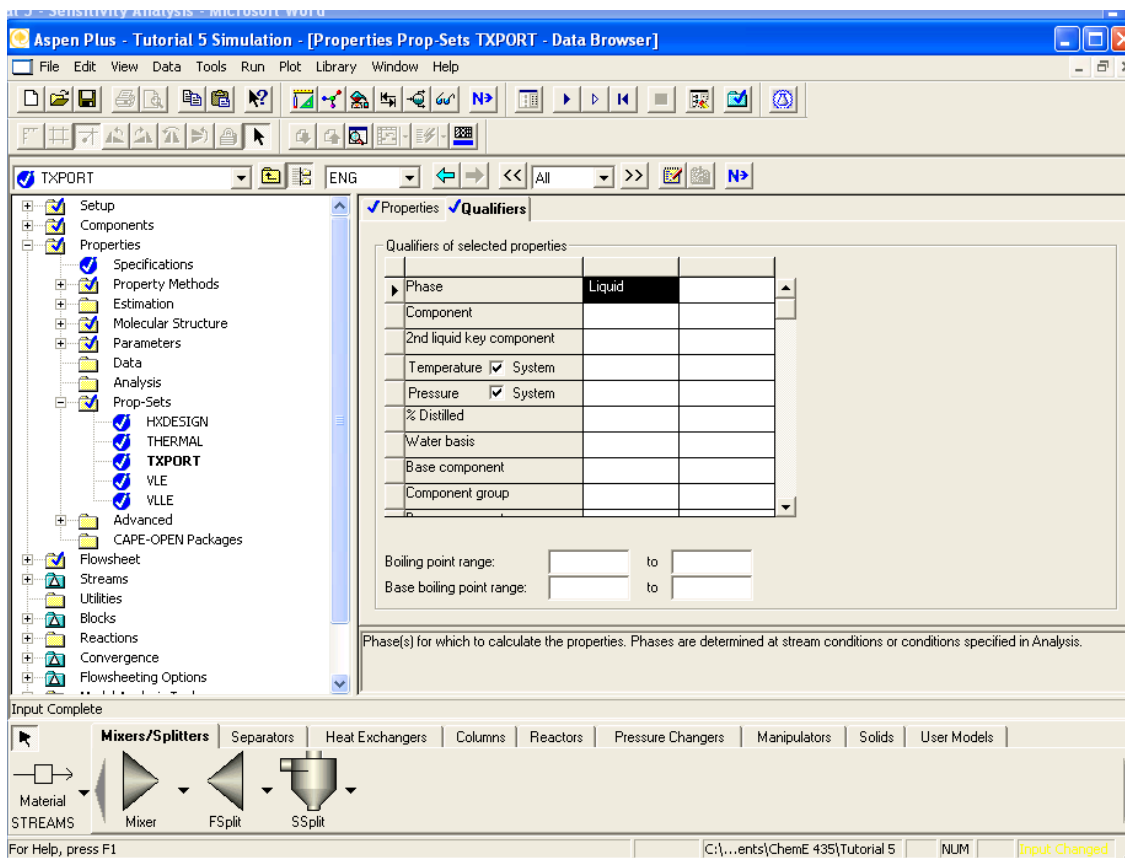
Figure 11: Qualifiers Window

We must now add the TXPORT property set to the stream table that is shown on the process flowsheet. To do this we must go to the Report Options window under the Setup tab in the Data Browser Window. Under the stream tab, hit the Property Sets button. This will open up the window shown in Figure 12.
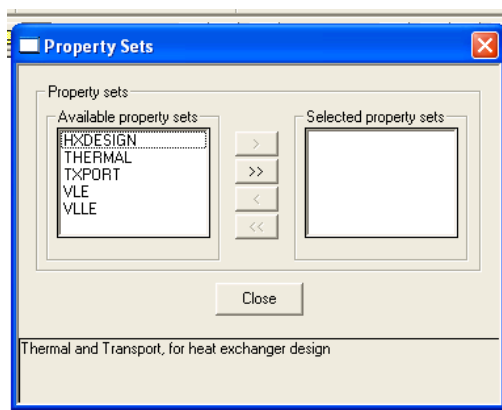
Figure 12: Property Sets Window

Select TXPORT and hit the single arrow button pointing to the right. This will move TXPORT to the side labeled Selected Property Sets, and it will now be displayed in the

stream table. After you have done this, close the Property Sets window. To reduce the number of variables shown in our stream table (to reduce its size), uncheck the mole flow basis box. This will remove the mole flows from the stream table (all of our assigned values have been mass flows so these have not played a role in our work yet). When you have done this, reinitialize and rerun your simulation. In order to have the changes to the stream table show up, you will most likely need to click on the stream table and then click off of it. Another option is to delete the existing stream table and add a new one to the process flowsheet. For comparison sake, my final stream table is shown below in Figure 13. Unfortunately, the diffusivity values (with the units of ft^2/hr) are too small to show differences in the table. However, if you were to switch the units from the default ones, you would get values that show differences in the three decimal places reported in the table.

| Tutorial5 - Sensitivity Analysis								
Stream ID		FEED	MIBK1	MIBK2	M-A1	M-A2	W-A1	WATER
Temperature	F	75.0	75.0	75.0	75.0	75.0	75.0	75.0
Pressure	psi	50.00	50.00	50.00	50.00	50.00	50.00	50.00
Vapor Frac		0.000	0.000	0.000	0.000	0.000	0.000	0.000
Mole Flow	lbmol/hr	3.636	0.998	0.899	1.938	1.204	2.696	2.392
Mass Flow	lb/hr	100.000	100.000	90.079	141.052	102.593	58.948	46.434
Volume Flow	cu ft/hr	1.825	2.009	1.809	2.772	2.029	1.011	0.767
Enthalpy	MMBtu/hr	-0.435	-0.140	-0.127	-0.246	-0.161	-0.329	-0.293
Mass Frac								
WATER		0.500			0.041	0.024	0.751	0.900
ACETONE		0.500			0.263	0.091	0.220	0.078
METHY-01			1.000	1.000	0.697	0.885	0.030	0.022
*** LIQUID PHASE ***								
Density	lb/cu ft	54.800	49.783	49.783	50.892	50.565	58.302	60.543
Viscosity	cP	0.720	0.552	0.552	0.498	0.542	0.851	0.907
Surface Ten	dyne/cm	61.235	23.538	23.538	31.578	29.101	68.595	71.528
DMX	sq ft/hr							
WATER		<0.001			<0.001	<0.001	<0.001	<0.001
ACETONE		<0.001			<0.001	<0.001	<0.001	<0.001
METHY-01			0.000	0.000	<0.001	<0.001	<0.001	<0.001

Figure 13: Final Stream Table

Next week: Separation Spreadsheets by Mark Burns, University of Michigan

Tutorial #5 Homework and Solution

Question:

What flow rate of MIBK is necessary to achieve 95% purity of the water stream? Show your results with the stream table from your simulation. Hint: Modify your existing design specification by changing both the target spec and the range for the independent variable (I suggest an upper limit of 400 lbs/hr). If your upper limit is not increased above the final result, your solution will not converge!

Solution:

From my Aspen simulation I obtained a feed rate of 324 lbs/hr MIBK, to get a water purity of 95 wt%. This answer may vary between Aspen simulations, but your results should be close to this (within 5 lbs/hr).

Tutorial 5 - Sensitivity Analysis								
Stream ID		FEED	MIBK1	MIBK2	M-A1	M-A2	W-A1	WATER
Temperature	F	75.0	75.0	75.0	75.0	75.0	75.0	75.0
Pressure	psi	50.00	50.00	50.00	50.00	50.00	50.00	50.00
Vapor Frac		0.000	0.000	0.000	0.000	0.000	0.000	0.000
Mole Flow	lbmol/hr	3.636	0.998	3.239	1.938	3.835	2.696	2.100
Mass Flow	lb/hr	100.000	100.000	324.409	141.052	344.063	58.948	39.295
Volume Flow	cuft/hr	1.825	2.009	6.517	2.772	6.826	1.011	0.641
Enthalpy	MMBtu/hr	-0.435	-0.140	-0.456	-0.246	-0.525	-0.329	-0.258
Mass Frac								
WATER		0.500			0.041	0.020	0.751	0.950
ACETONE		0.500			0.263	0.034	0.220	0.030
METHY-01			1.000	1.000	0.697	0.946	0.030	0.020
*** LIQUID PHASE ***								
Density	lb/cuft	54.800	49.783	49.783	50.892	50.407	58.302	61.333
Viscosity	cP	0.720	0.552	0.552	0.498	0.564	0.851	0.924
Surface Ten	dyne/cm	61.235	23.538	23.538	31.578	28.470	68.595	72.376
DMX	sqft/hr							
WATER		< 0.001			< 0.001	< 0.001	< 0.001	< 0.001
ACETONE		< 0.001			< 0.001	< 0.001	< 0.001	< 0.001
METHY-01			0.000	0.000	< 0.001	< 0.001	< 0.001	< 0.001

Aspen Tutorial #6: Aspen Distillation

Outline:

- Problem Description
- Aspen Distillation Options
- DSTWU Distillation
- RadFrac Distillation

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 the various distillation calculation methods that Aspen uses. We will be completing the separation of our acetone/MIBK streams based on one of the simplified distillation methods, DSTWU and one of the more rigorous distillation calculation methods, RadFrac. From this we will be able to compare the results of the two distillation methods.

Aspen Distillation Options:

Aspen has multiple unit operations options for completing distillation problems, based on the complexity of the user's application. Open up your existing Aspen simulation and click on the Separators tab in the Equipment Model Library. In this tab you will see the first option that users can choose for completing a distillation process, SEP2. This unit operation can be used to model separation processes with only two possible outlet streams. This process can be used to simulate distillations, but it does not provide the level of detail that is available when using some of the other distillation options. Some key variables it does not consider include the number of trays and the reflux ratio. For this reason this option is not recommended except as a very general screening process.

Now select the Columns tab in the Equipment Model Library. You will notice a number of distillation column options. This tutorial will focus on introducing you to the three general distillation choices, DSTWU, Distl, and RadFrac. The other six unit operation choices complete much more rigorous calculations than we require for our application and they are intended for use in more difficult separations and specific applications (i.e. PetroFrac is used in simulating refining processes).

The DSTWU unit operation is designed for single feed, two product distillation processes. This column completes calculations using Gilliland's, Winn's, and Underwood's methods for calculations of stages and reflux ratios as indicated in Table 1. These calculations are completed based on two assumptions, constant molar overflow and constant relative volatilities.

Table 1: DSTWU Calculation Methods

Shortcut Method	Calculates For:
Winn	Minimum number of stages
Underwood	Minimum reflux ratio
Gilliland	Required reflux ratio for a specified number of stages or required number of stages for a specified reflux ratio

For a specified product recovery (both light and heavy), the DSTWU column first estimates the minimum number of stages and the minimum reflux ratio, and then it calculates the either the required reflux ratio or the required number of theoretical stages based on the user input. During these calculations, Aspen will also estimate the optimum feed stage location and the condenser and reboiler duties. Finally, when the calculations are complete, Aspen can produce tables and plots of the reflux ratio/stage profile. When completing complicated simulations later in your career, you could use this column to get a quick idea about a process, and use its results as inputs to a more detailed simulation.

The Distl unit operation is also designed for a single feed, two product distillation process. However, this column calculates product compositions based on the Edmister approach. Again, the calculations are completed based on the assumptions of constant molar overflow and constant relative volatilities. The user is required to input a number of the column specifications with this unit operation, including the number of stages, the reflux ratio, and the distillate to feed ratio. We will not be using this option.

The final general distillation unit operation is the RadFrac column. This distillation unit completes much more rigorous calculations than the other two methods and can be used to simulate absorption, stripping, extractive distillation, and azeotropic distillation for solids, liquids, and gases. This column can also be used for highly non-ideal liquid solutions or processes with an on-going chemical reaction. Finally, the RadFrac column can have multiple feed and product streams (including pump-around streams) and it can simulate columns with trays, random packing, or structured packing. As you can see, this distillation option is much more complicated than the previous two methods, and we will be covering this method in more depth as we input the data for it.

DSTWU Distillation:

In the last Aspen homework, we adjusted our design specification input in Tutorial #5 to achieve a water purity of 95%. We will keep this updated specification in our ongoing simulation, so if you did not complete the homework two weeks ago, do so now.

The first update we will make to our simulation is the addition of another mixer. Add in a new mixer which combines the two streams of acetone and MIBK from the two flash separators that we added in the previous tutorials. This can be seen in the process flowsheet window shown in Figure 1.
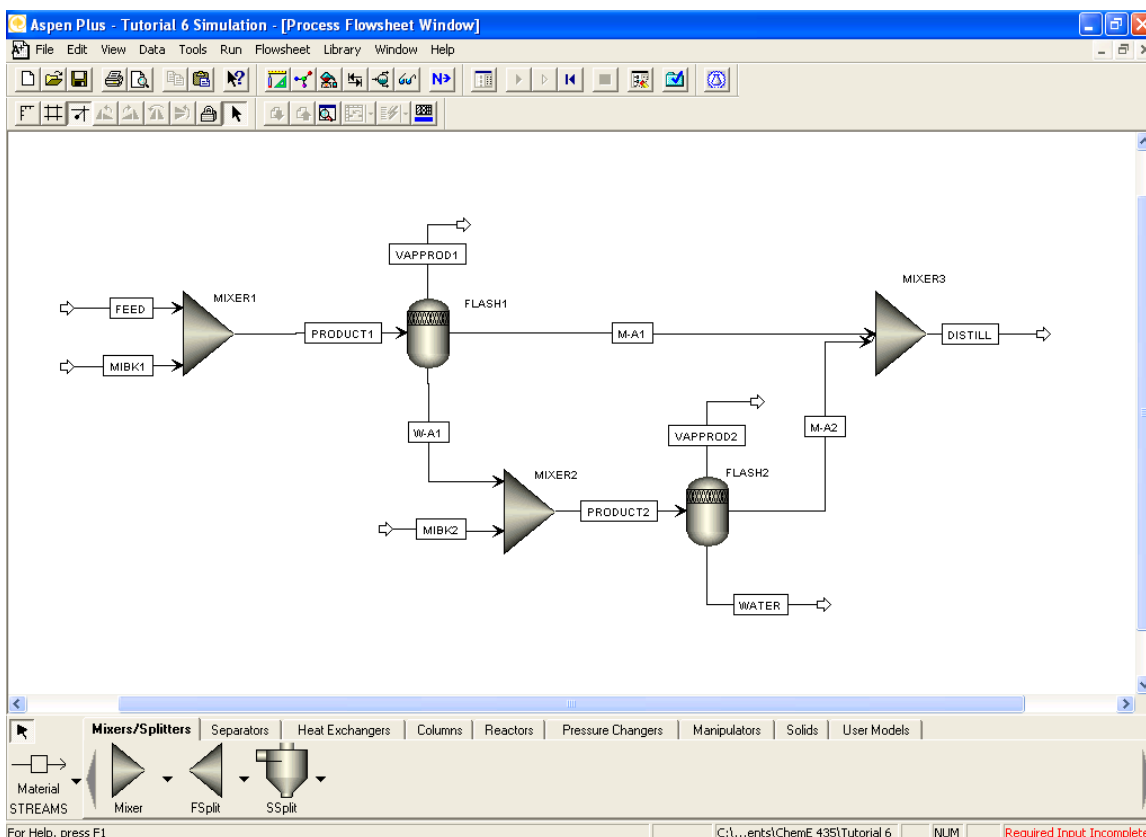
Aspen Tutorial #6

Figure 1: Acetone/MIBK Mixer

At this point save your Aspen simulation under two names. We will use one version to complete a distillation with the DSTWU distillation column and we will use the other version to complete the simulation with the RadFrac column. I would suggest saving them with names that indicate which distillation method is being used.

Now select the Columns tab in the Equipment Model Library and place a DSTWU column into the process flowsheet window. Connect the product stream from the new mixer to the DSTWU column and add in two product streams where Aspen indicates they are required. We will also be adding in a third product stream off of the condenser, to account for any free water product that can be separated from within the condenser. Rename the streams and column as you see fit. At this point your flowsheet should look similar to that in Figure 2.
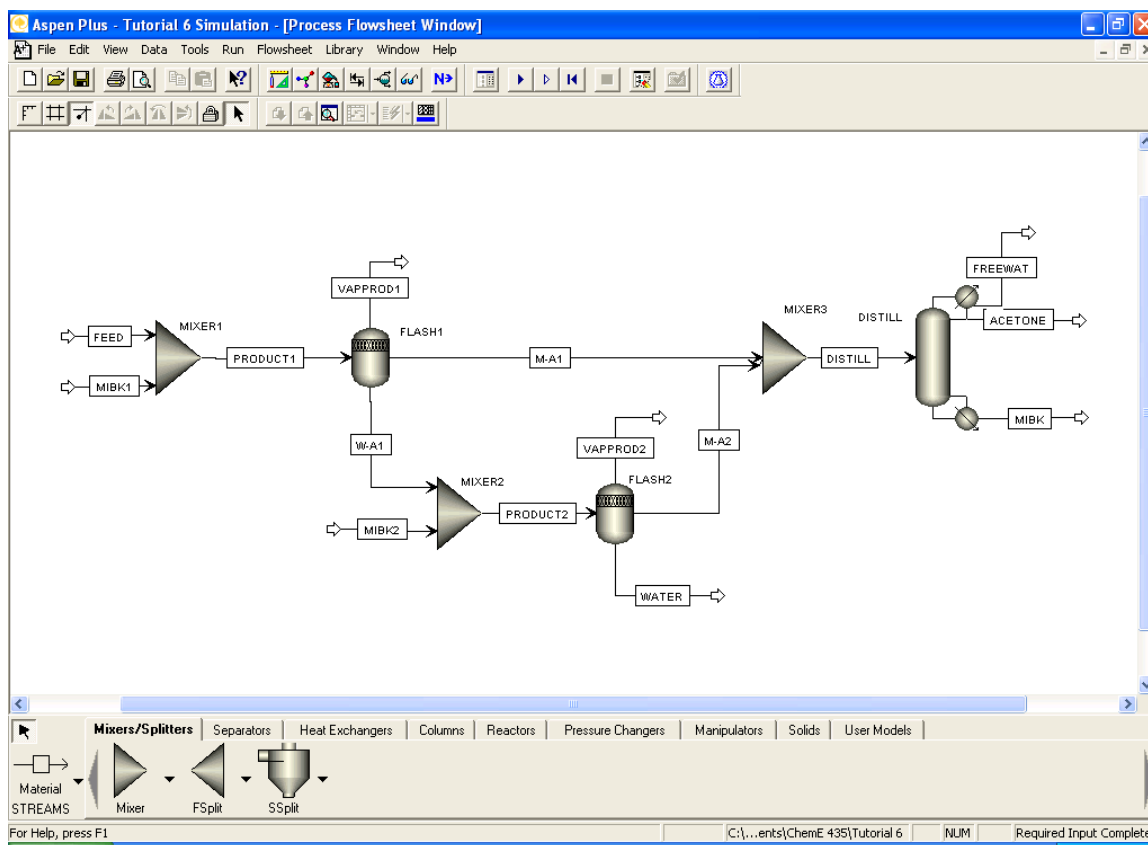
Figure 2: Completed Process Flowsheet

Now open up the Data Browser window. You will notice that we are only required to update our data input in the Blocks tab. Under the appropriate option for the new mixer, input a mixing temperature and pressure of 75º F and 50 psi. Then open up the appropriate option for the distillation column. The input window is shown below in Figure 3.
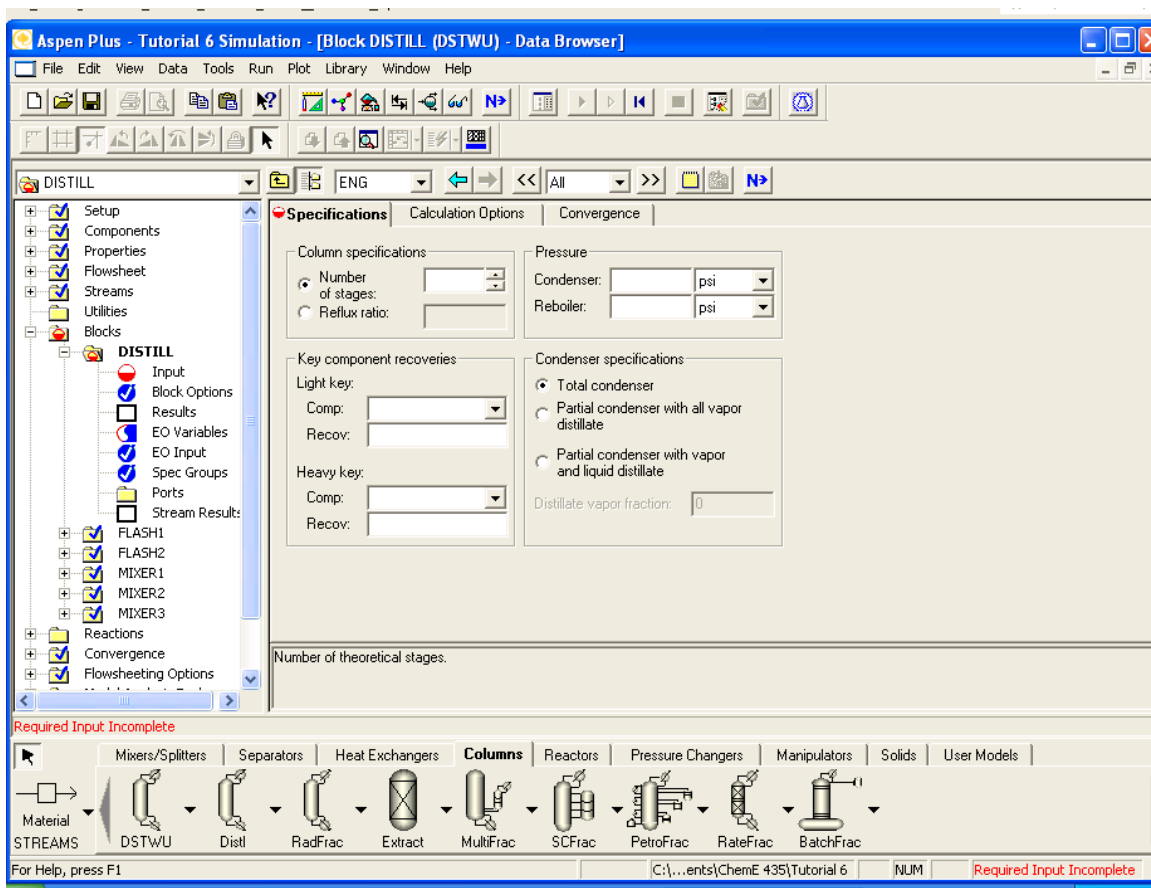
Figure 3: DSTWU Data Input Window

For this simulation we will be inputting the reflux ratio, the key component recoveries, and the tower pressures. For our purposes, we will assume that the tower has no pressure drop throughout it. However, we will set the condenser and reboiler pressures to 15 psi to aid in our separation process. We will start with an input reflux ratio of 1.5, but we will be varying this value to try and get our desired product purity. The component recovery values that are input are equal to the amount of each component in the distillate divided by the amount of each component in the feed. For this reason a recovery of 99% for acetone and 1% for the MIBK are not unreasonable if our distillation tower is operating well. The completed input screen is shown in Figure 4.
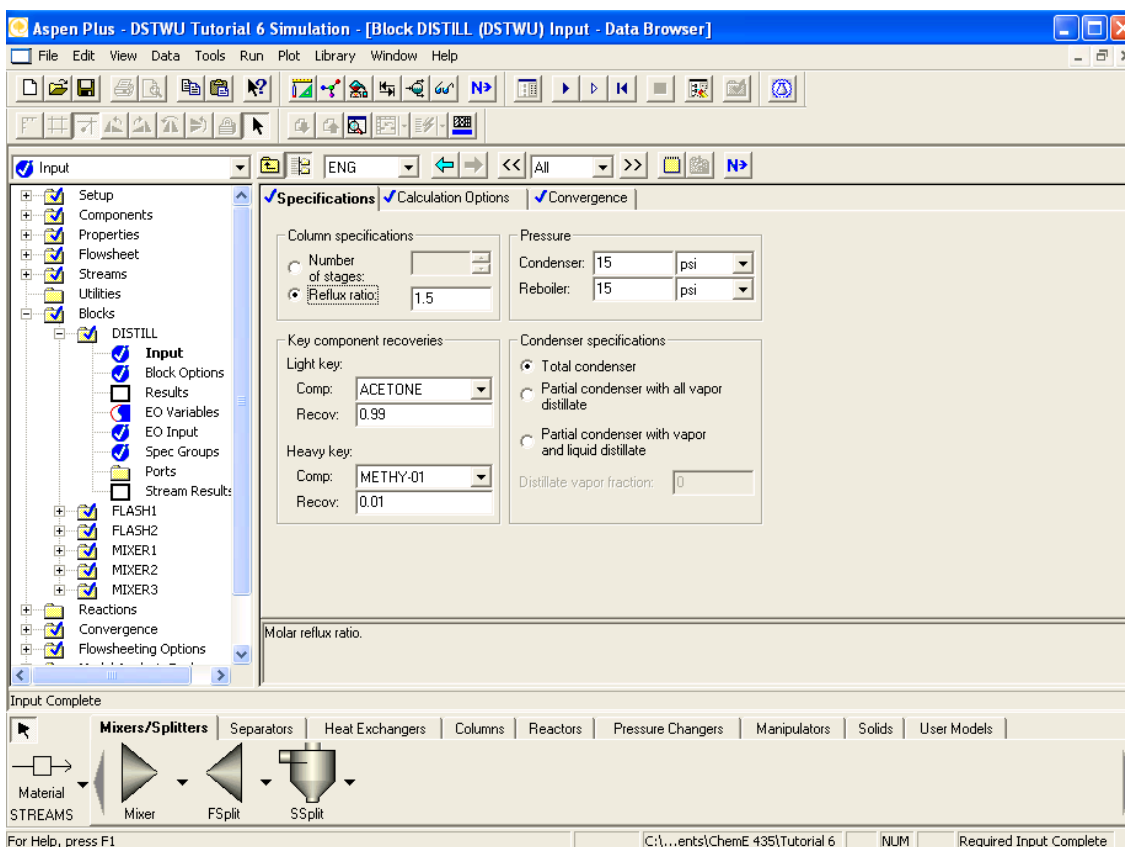
Figure 4: Completed DSTWU Input Window

For our benefit, we would also like Aspen to produce a table of reflux ratio vs. the total number of calculated theoretical trays. This can be easily done by selecting the Calculation Options tab at the top of the DSTWU input window. Check the box corresponding to this calculation now.

At this point our simulation is complete. Reinitialize and run your simulation. If you look closely at your results, you will notice that we do not achieve the desired 90% purity of acetone in this simulation. The stream table from my simulation is shown in Figure 5 where it can be seen that my simulation only achieved an acetone purity of 88%.

We can examine the reflux ratio profile for our distillation column at this time. This can be done by opening up the Data Browser window (if it is not already open) and selecting the Blocks tab. Under this tab there is an option labeled Results. Open up this window, and then select the tab at the top entitled Reflux Ratio Profile. If you were designing this tower, you could use the information in this table to determine the most cost-effective design for your distillation column. Each tray will add to the equipment cost, while the increased reflux adds to the operating costs of the column. We will use some of this information in our input for the RadFrac column.

Tutorial 6 - DSTWU Distillation					
Stream ID		DISTILL	ACETONE	MIBK	FREEWAT
Temperature	F	75.2	137.0	235.2	137.0
Pressure	psi	50.00	15.00	15.00	15.00
Vapor Frac		0.000	0.000	0.000	0.000
Mole Flow	lbmol/hr	5.774	1.006	4.253	0.514
Mass Flow	lb/hr	485.182	54.950	420.966	9.266
Volume Flow	cuft/hr	9.586	1.161	9.474	0.151
Enthalpy	MMBtu/hr	-0.771	-0.109	-0.560	-0.063
Mass Flow	lb/hr				
WATER		12.666	2.367	1.033	9.266
ACETONE		48.835	48.346	0.488	
METHY-01		423.681	4.237	419.445	
Mass Frac					
WATER		0.026	0.043	0.002	1.000
ACETONE		0.101	0.880	0.001	
METHY-01		0.873	0.077	0.996	

Figure 5: Initial DSTWU Results

Because we did not achieve the desired product purity, we will now write a design spec to try and reach our goal. Under the Flowsheeting Options tab select Design Spec and add a new one. This spec will be the calculation of the mass fraction of acetone in the acetone product stream. We will try to achieve our desired 90 wt% by varying the molar reflux ratio of the column between 0.5 and 5.0. Specify a tolerance of 0.5% for this spec. If you do not remember how to do this, refer to Tutorial #5. Hint: the reflux ratio is a Block-Var.

After you have input your design spec, rerun your simulation. In doing so, you should get an error that your Aspen simulation did not converge. Close this error message by hitting the cancel button. Because of the simplifications that are used in this type of distillation column, the purity level of our product is not affected by the reflux ratio. This can be confirmed by looking at the Convergence tab in the Data Browser window. Under this option one of the two solver files should have a red x through it. Opening up this option and selecting the Spec History tab will open up the window shown in Figure 6. You will notice in this window that the error values shown in the table do not change as the reflux ratio does, indicating that our dependent variable value is not changing.

This step was completed to provide a warning to you in your future simulation efforts. While some of the shortcut methods appear to provide a quick way to obtain results, they do not always work or provide the accuracy that is desired. For this reason we will complete the same calculations with the RadFrac column to see if the results are any different.
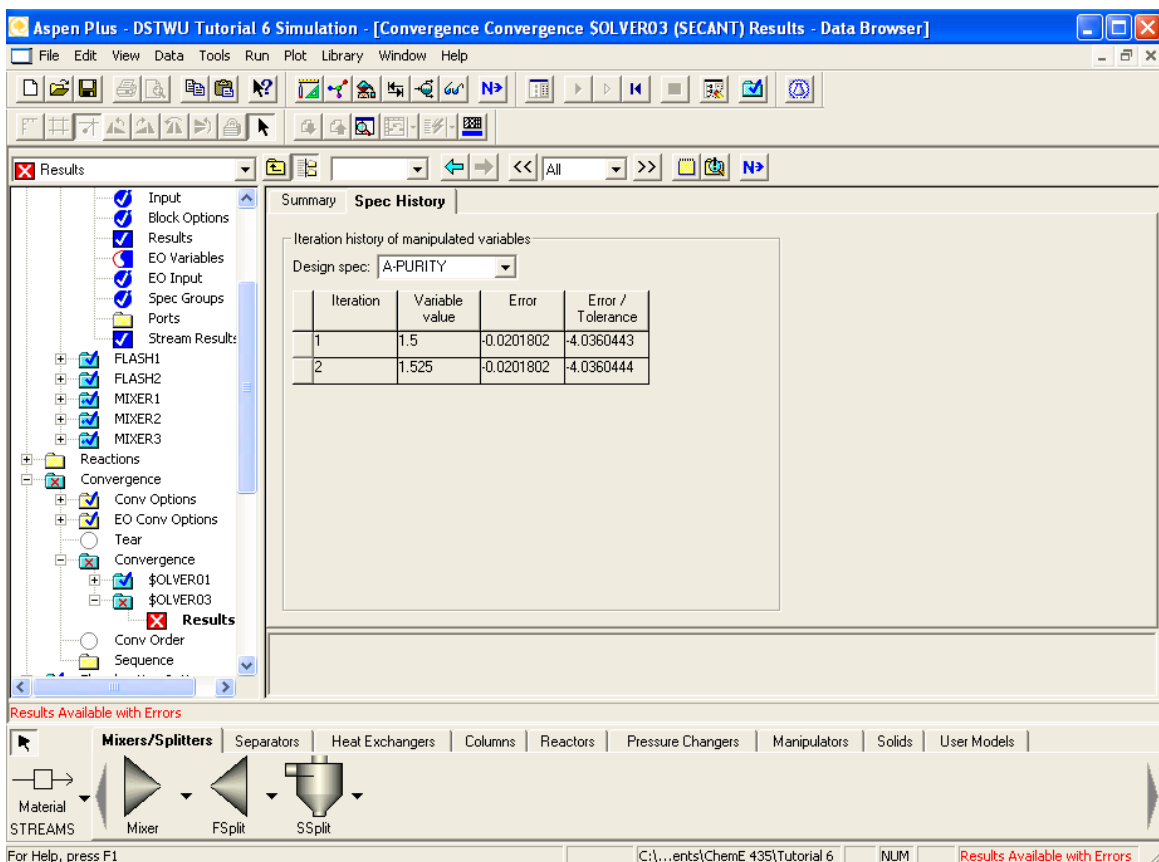
Figure 6: Convergence Window

RadFrac Distillation:

Close your simulation with the DSTWU distillation column and open up the second version that you should have saved earlier in this tutorial. Add in a RadFrac distillation column and three product streams as we did earlier. Your process flowsheet should again look similar to that seen in Figure 2.

Now open up the Data Browser window and the Blocks option. Input the same process design conditions for the mixer and then open up the screen related to our new column. This input window is shown in Figure 7. As you can see, this column requires a lot more input than the DSTWU column required.

Figure 7: RadFrac Input Window

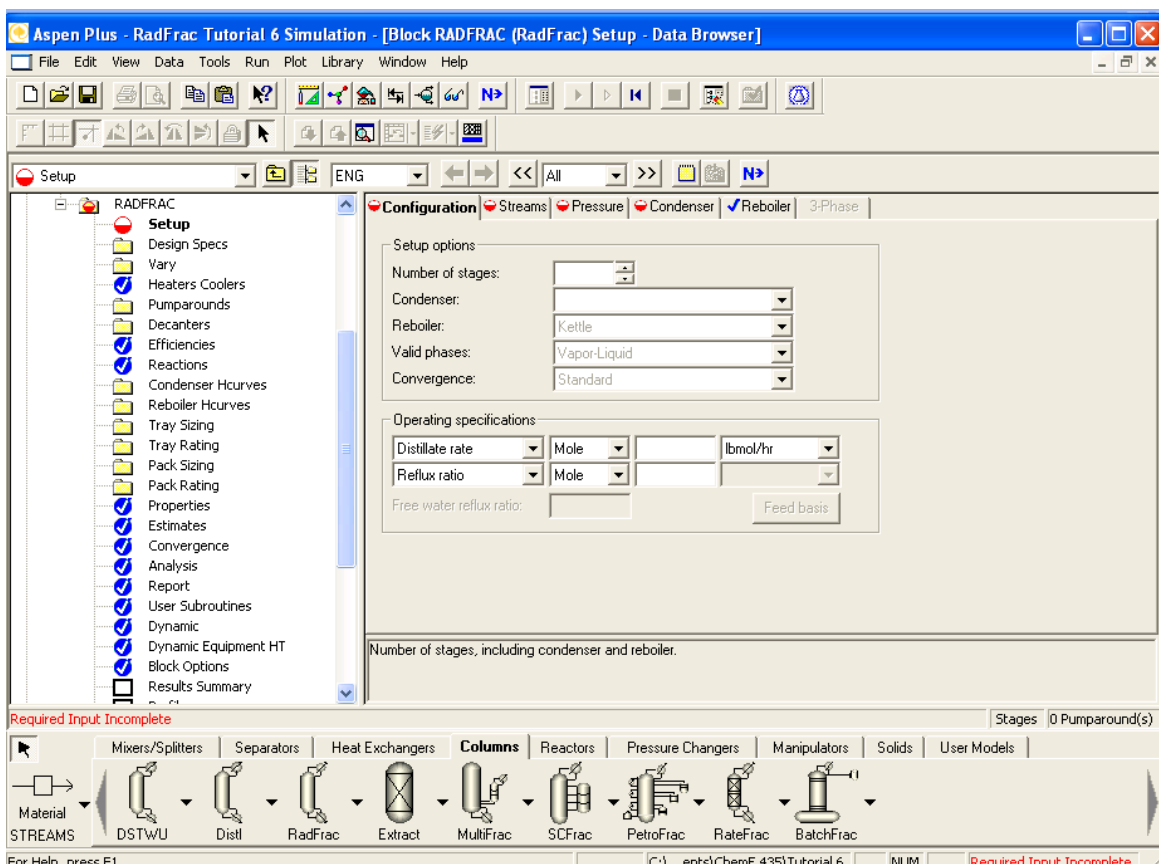In order to compare the two distillation methods, we must input identical values into this input window wherever possible. In the Configuration tab select a total condenser, and change the valid phases to Vapor-Liquid-FreeWaterCondenser. Input a reflux ratio of 1.5 as well (molar basis). In order for us to input a specified product recovery, we must change one of the operating specifications to the option Distillate to feed ratio. However, this option is different than that for the DSTWU column and we must select the specific components that we are specifying the recovery of. To do this hit the Feed Basis button. Move acetone from the available list to the selected list under the components box and then hit the close button. Now input a recovery of 0.99. At this point we have input all of the data that was required of us for the DSTWU column (for this window), but in this case Aspen still requires more data.

You might remember looking at the reflux ratio to theoretical tray profile in the DSTWU simulation. In this profile, Aspen had calculated that 10 theoretical trays were required for a reflux ratio of 1.49. For this reason, we will input 10 trays into this simulation. At this point the input for the Configuration tab should be complete and your window should look like that seen in Figure 8.
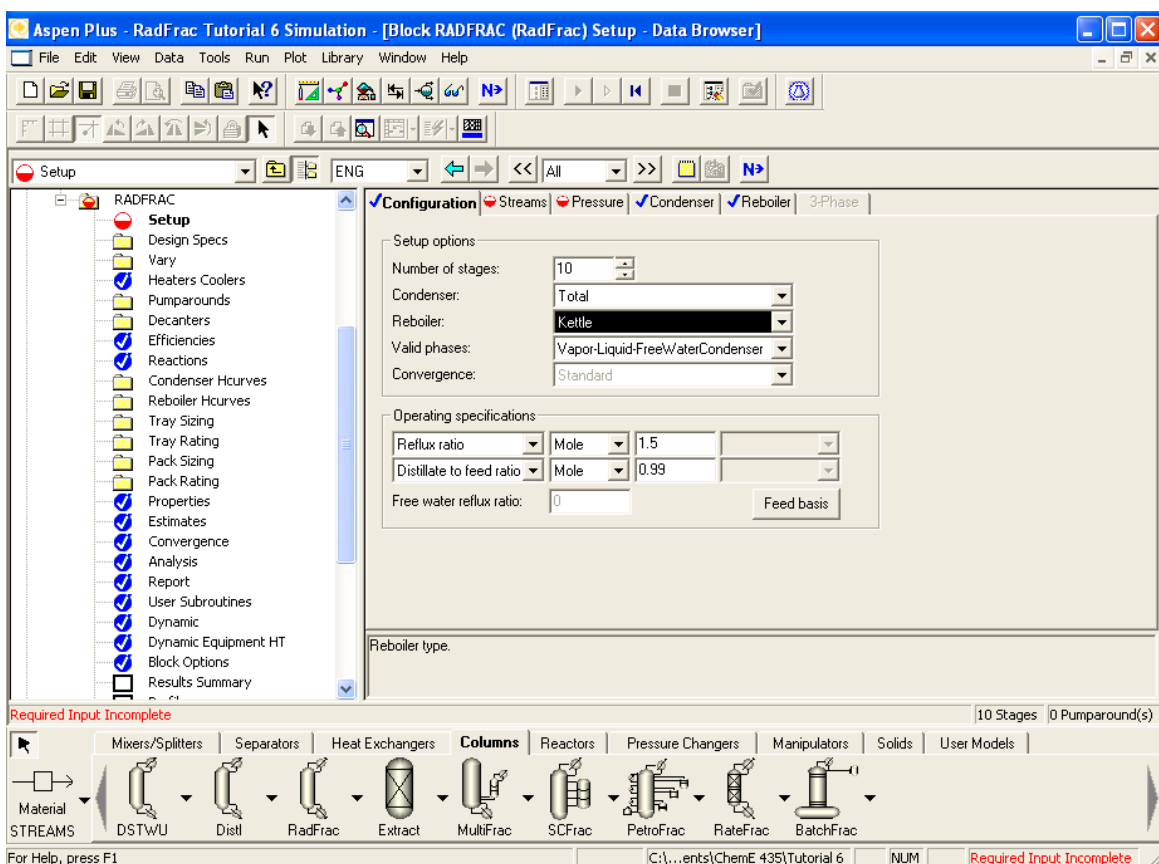
Aspen Tutorial #6

Figure 8: Completed Configuration Input

Under the Streams tab we need to input the location of the feed stream. As discussed in you mass transfer class, we will put the feed at the middle stage of the column, tray 5. In addition, your acetone stream should say 1st liquid, your water stream should say free water, and your MIBK stream should say liquid. This completes the Streams tab input. You might notice that the tray corresponding to each product stream is shown in this window. If we had any side draws from our tower or additional feeds, we would need to input which tray they occur from or to in this window.

In the final input tab, Pressure, we use the same assumption that we used in the DSTWU simulation, no pressure drop. Again, we will simulate a distillation column that is operating at 15 psi. Input this as the operating pressure at Stage 1.

At this point our required input is again complete and we are ready to run our simulation. Reinitialize and run your simulation at this point. You will notice in Figure 9 that this initial simulation actually calculates a worse purity for our acetone product than that which was obtained with the DSTWU distillation column. For this reason we will again try to input a design spec to see if we can achieve our desired 90% purity. Input the same design spec that we used in the DSTWU distillation simulation and then reinitialize and rerun your simulation.

Tutorial 6 - RadFrac Distillation					
Stream ID		DISTILL	ACETONE	FREEWAT	MIBK
Temperature	F	75.2	138.6	138.6	213.1
Pressure	psi	50.00	15.00	15.00	15.00
Vapor Frac		0.000	0.000	0.000	0.000
Mole Flow	lbmol/hr	5.774	0.832	0.354	4.587
Mass Flow	lb/hr	485.182	46.466	6.379	432.336
Volume Flow	cuft/hr	9.586	0.980	0.104	9.518
Enthalpy	MMBtu/hr	-0.771	-0.091	-0.043	-0.601
Mass Flow	lb/hr				
WATER		12.666	2.021	6.379	4.266
ACETONE		48.835	38.224		10.611
METHY-01		423.681	6.222		417.460
Mass Frac					
WATER		0.026	0.043	1.000	0.010
ACETONE		0.101	0.823		0.025
METHY-01		0.873	0.134		0.966

Figure 9: Initial RadFrac Results

This time your simulation should converge, with an acetone weight percent of 90%. The results that I obtained are shown below in Figure 10.

Tutorial 6 - RadFrac Distillation					
Stream ID		DISTILL	ACETONE	FREEWAT	MIBK
Temperature	F	75.2	136.5	136.5	208.0
Pressure	psi	50.00	15.00	15.00	15.00
Vapor Frac		0.000	0.000	0.000	0.000
Mole Flow	lbmol/hr	5.774	0.832	0.234	4.707
Mass Flow	lb/hr	485.182	45.126	4.219	435.837
Volume Flow	cuft/hr	9.586	0.954	0.069	9.532
Enthalpy	MMBtu/hr	-0.771	-0.090	-0.029	-0.618
Mass Flow	lb/hr				
WATER		12.666	1.938	4.219	6.509
ACETONE		48.835	40.596		8.239
METHY-01		423.681	2.592		421.089
Mass Frac					
WATER		0.026	0.043	1.000	0.015
ACETONE		0.101	0.900		0.019
METHY-01		0.873	0.057		0.966

Figure 10: Final RadFrac Results

As discussed in Tutorial #2, we should now check our results to make sure that they are reasonable. We will also check some of the operating parameters for the distillation column. If you look at the Run Control Panel, you will notice that the second design spec that we used took 5 iterations to converge, which is quite reasonable. Now open up the Data Browser window if it is not already open. We will look closely at the results for the

Aspen Tutorial #6

RadFrac column because this is the only significant addition to our simulation since the last time we checked the results closely. Select the appropriate unit operation under the Blocks option. Scroll down until you see the choice Results Summary and open this window. This is shown in Figure 11.
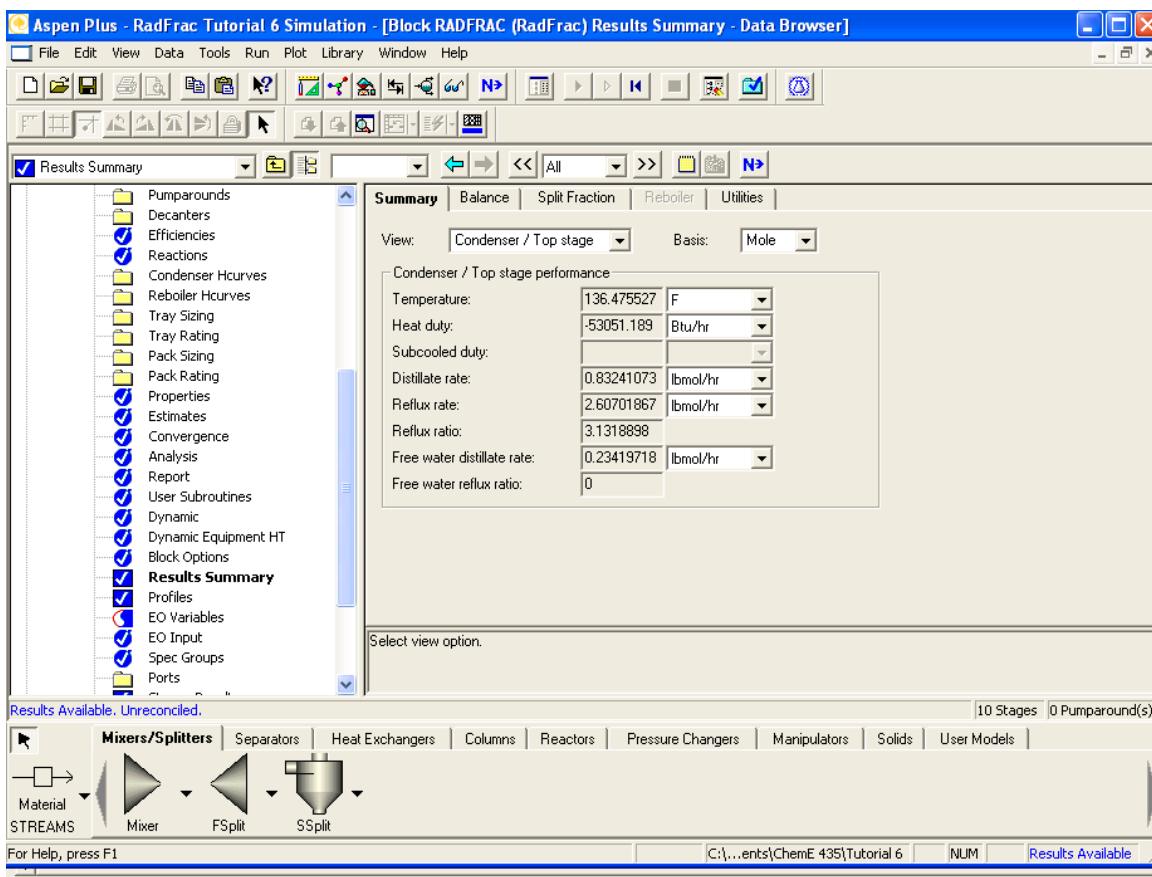

Figure 11: RadFrac Results Summary

This window shows the final operating conditions for the distillation column that were calculated by the program. You can see in this window that our final molar reflux ratio was 3.13. You can also see the required condenser cooling duty. If you switch to the Reboiler / Bottom stage option you can see the required heat input into this column as well.

If you select the Balance tab at the top of the screen, you can see the overall heat and material balances for the column. You can also see the relative difference in the values (emphasizing the fact that no simulation is "perfect").

Under the Profiles option (in the Data Browser options) Aspen presents you with a summary of the operating conditions for this simulation. Under the TPFQ option you can see a breakdown of the liquid and vapor flow rates from each tray. You can also modify the table to show the heat balance or temperature profile. Under the Compositions tab at the top of the screen, you can see a profile of each of the components throughout the

column. If all of your checks appear to be acceptable, you have finished your final Aspen tutorial.

Next Week: Stand-alone Aspen Problem

Hints for next week's final Aspen homework problem:

- Use DSTWU to determine the minimum reflux ratio and number of stages. Under View/Reports, you can generate a report for a DSTWU column that shows this information (if the inputs are correct).

- An input reflux ratio of -1 causes Aspen to use the minimum reflux ratio. Any negative number input as a reflux ratio is used as that number times the minimum reflux ratio (i.e. -2 indicates a reflux ratio of $2*R_{min}$).

- Tables in the Data Browser window can be plotted by selecting each column one at a time and then selecting Plot/X-Axis Variable (or Y-Axis Variable). After each axis variable has been selected the graph can be plotted with Plot/Display Plot.

Tutorial #6 Homework and Solution

Question:

Submit a copy of the Input Summary that is generated for your RadFrac distillation simulation and a stream table with the four final product streams only (two water streams, an acetone stream, and an MIBK stream). For help doing this, see Tutorial #2.

Solution:

;Input Summary created by Aspen Plus Rel. 12.1 at 09:37:13 Tue Nov 16, 2004
;Directory   Filename C:\DOCUME~1\Matt\LOCALS~1\Temp\~ap1a.tmp

TITLE 'Tutorial 6 - RadFrac Distillation'

IN-UNITS ENG

DEF-STREAMS CONVEN ALL

DESCRIPTION "THIS IS THE SOLUTION, DO NOT USE ME"
   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

SOLVE
   PARAM METHOD=EO

FLOWSHEET
   BLOCK MIXER1 IN=FEED MIBK1 OUT=PRODUCT1
   BLOCK FLASH1 IN=PRODUCT1 OUT=VAPPROD1 M-A1 W-A1
   BLOCK MIXER2 IN=W-A1 MIBK2 OUT=PRODUCT2

```
    BLOCK FLASH2 IN=PRODUCT2 OUT=VAPPROD2 M-A2 WATER
    BLOCK MIXER3 IN=M-A1 M-A2 OUT=DISTILL
    BLOCK RADFRAC IN=DISTILL OUT=ACETONE MIBK FREEWAT

PROPERTIES NRTL

PROP-DATA NRTL-1
    IN-UNITS ENG
    PROP-LIST NRTL
    BPVAL WATER ACETONE .0544000000 755.9488740 .3000000000 0.0  &
        0.0 0.0 68.00000346 203.1800024
    BPVAL ACETONE WATER 6.398100000 -3256.183774 .3000000000  &
        0.0 0.0 0.0 68.00000346 203.1800024
    BPVAL WATER METHY-01 9.162943000 -2247.739182 .2000000000  &
        0.0 0.0 0.0 32.00000374 240.8000021
    BPVAL METHY-01 WATER -3.230481000 2175.978583 .2000000000  &
        0.0 0.0 0.0 32.00000374 240.8000021
    BPVAL ACETONE METHY-01 -5.445200000 3300.340834 .3000000000  &
        0.0 0.0 0.0 77.00000338 230.2340022
    BPVAL METHY-01 ACETONE 5.301300000 -3124.634735 .3000000000  &
        0.0 0.0 0.0 77.00000338 230.2340022

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.
    MASS-FRAC METHY-01 1.

STREAM MIBK2
    SUBSTREAM MIXED TEMP=75. PRES=50. MASS-FLOW=50.
    MASS-FRAC METHY-01 1.

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

BLOCK MIXER2 MIXER
    PARAM PRES=50. T-EST=75.

BLOCK MIXER3 MIXER

BLOCK FLASH1 FLASH3
    PARAM TEMP=75. PRES=50.
```

BLOCK FLASH2 FLASH3
  PARAM TEMP=75. PRES=50.

BLOCK RADFRAC RADFRAC
  PARAM NSTAGE=10 NPHASE=2
  COL-CONFIG CONDENSER=TOTAL
  FEEDS DISTILL 5
  PRODUCTS ACETONE 1 L1 / FREEWAT 1 W / MIBK 10 L
  P-SPEC 1 15.
  COL-SPECS D:F=0.99 RW=0. MOLE-RR=1.5
  DB:F-PARAMS COMPS=ACETONE
  BLOCK-OPTION FREE-WATER=YES

DESIGN-SPEC A-PURITY
  DEFINE ACETON MASS-FRAC STREAM=ACETONE SUBSTREAM=MIXED &
    COMPONENT=ACETONE
  SPEC "ACETON" TO "0.90"
  TOL-SPEC "0.005"
  VARY BLOCK-VAR BLOCK=RADFRAC VARIABLE=MOLE-RR &
    SENTENCE=COL-SPECS
  LIMITS "0.5" "5.0"

DESIGN-SPEC W-PURITY
  DEFINE WATER MASS-FRAC STREAM=WATER SUBSTREAM=MIXED &
    COMPONENT=WATER
  SPEC "WATER" TO "0.95"
  TOL-SPEC "0.001"
  VARY MASS-FLOW STREAM=MIBK2 SUBSTREAM=MIXED &
    COMPONENT=METHY-01
  LIMITS "25" "400"

EO-CONV-OPTI

STREAM-REPOR WIDE NOMOLEFLOW MASSFLOW MASSFRAC
;

Aspen Tutorial #6

| Tutorial 6 - RadFrac Distillation					
Stream ID		WATER	FREEWAT	ACETONE	MIBK
Temperature	F	75.0	136.5	136.5	208.0
Pressure	psi	50.00	15.00	15.00	15.00
Vapor Frac		0.000	0.000	0.000	0.000
Mole Flow	lbmol/hr	2.100	0.234	0.832	4.707
Mass Flow	lb/hr	39.294	4.219	45.126	435.837
Volume Flow	cuft/hr	0.641	0.069	0.954	9.532
Enthalpy	MMBtu/hr	-0.258	-0.029	-0.090	-0.618
Mass Flow	lb/hr				
WATER		37.334	4.219	1.938	6.509
ACETONE		1.165		40.596	8.239
METHY-01		0.795		2.592	421.089
Mass Frac					
WATER		0.950	1.000	0.043	0.015
ACETONE		0.030		0.900	0.019
METHY-01		0.020		0.057	0.966

Final Homework and Solution

Question:

A total of 100 lb-mol per hour of a 40 mol% methanol and 60 mol% water mixture is to be separated at 1 atm to give a distillate that contains 92 mol% methanol and a bottom product that contains 4 mol% methanol. A total condenser is to be used and the reflux will be returned to the column as a saturated liquid at its bubble point. An operating reflux ratio of 1.5 times the minimum will be used. The feed is introduced into the column as a saturated liquid at its bubble point. Use Aspen Plus to complete the following: (a) generate a Txy diagram for the water-methanol system at 1 atm, (b) determine the minimum number of theoretical stages, (c) determine the minimum reflux ratio, (d) determine the heat loads of the condenser and reboiler for the condition of minimum reflux, (e) determine the quantities of the distillate and bottom streams using the actual reflux ratio, (f) determine the actual number of theoretical stages, (g) determine the heat load of the condenser for the actual reflux ratio, (h) generate a plot of the temperature profile and composition profile as a function of stage number (for both methanol and water).

Solution:

(a) From Aspen:
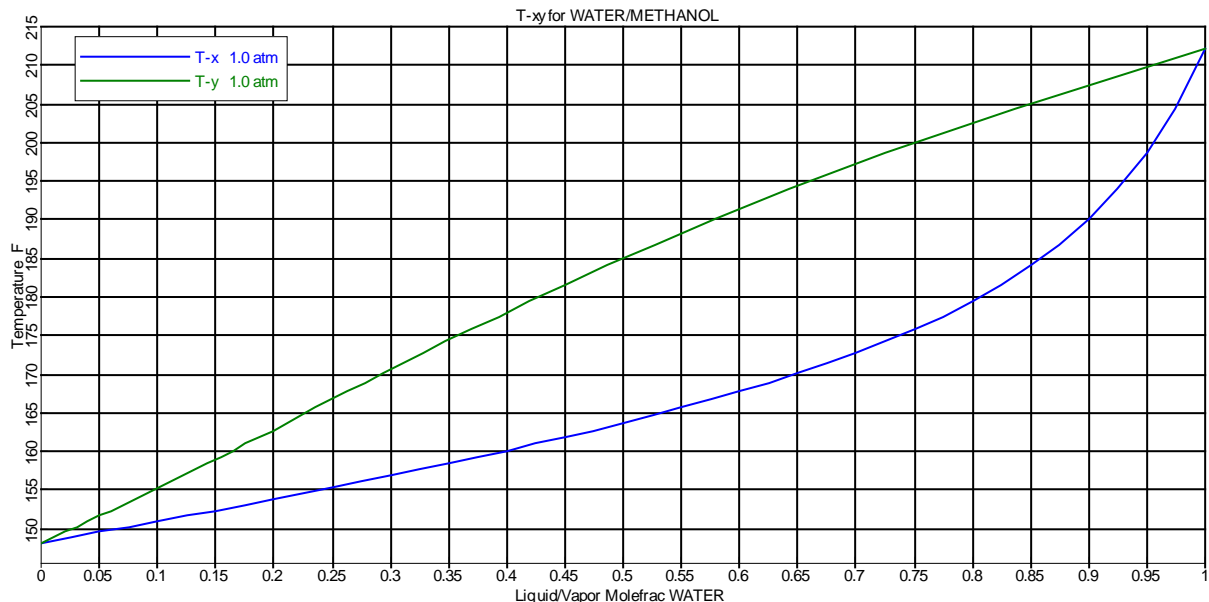
(b) The minimum number of theoretical stages is equal to 4.06 stages per a DSTWU simulation.

(c) The minimum molar reflux ratio is 0.504 per a DSTWU simulation.

(d) At minimum reflux, the condenser duty is ~951,298 BTU/hr and the reboiler duty is ~989,263 BTU/hr (from a DSTWU simulation).

(e) The actual distillate rate is 41.1 lbmol/hr and the actual bottoms rate is 58.9 lbmol/hr from a RadFrac simulation.

(f) The actual number of theoretical stages is 8 stages per a RadFrac simulation.

(g) The heal load for the condenser at the actual operation conditions is 1,114,319 BTU/hr per a RadFrac simulation.

(h) From a RadFrac simulation:
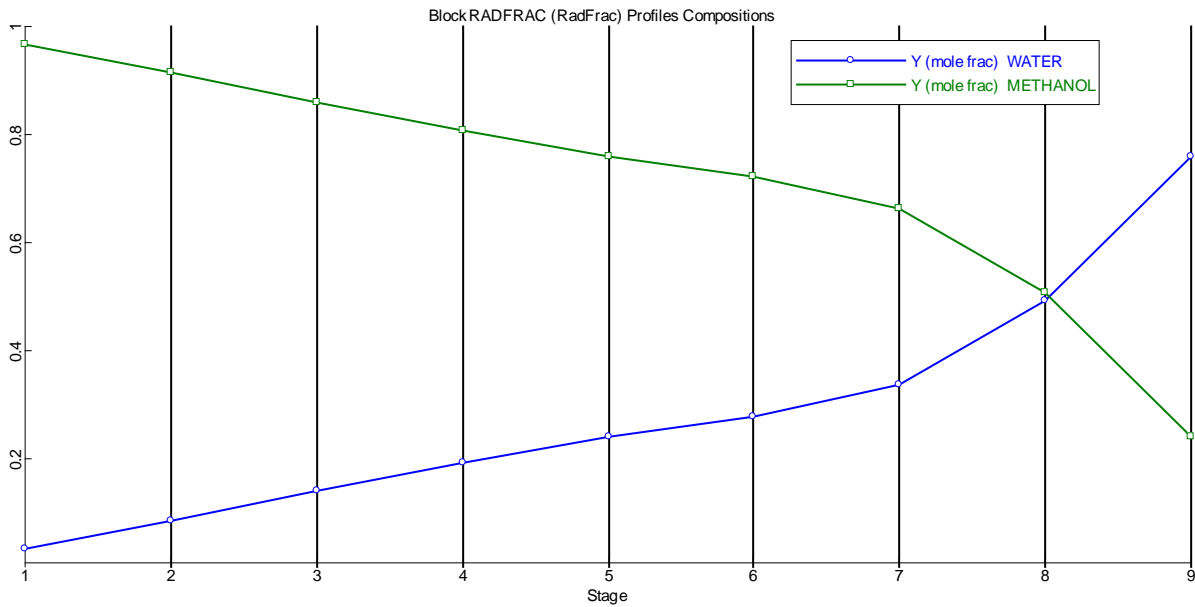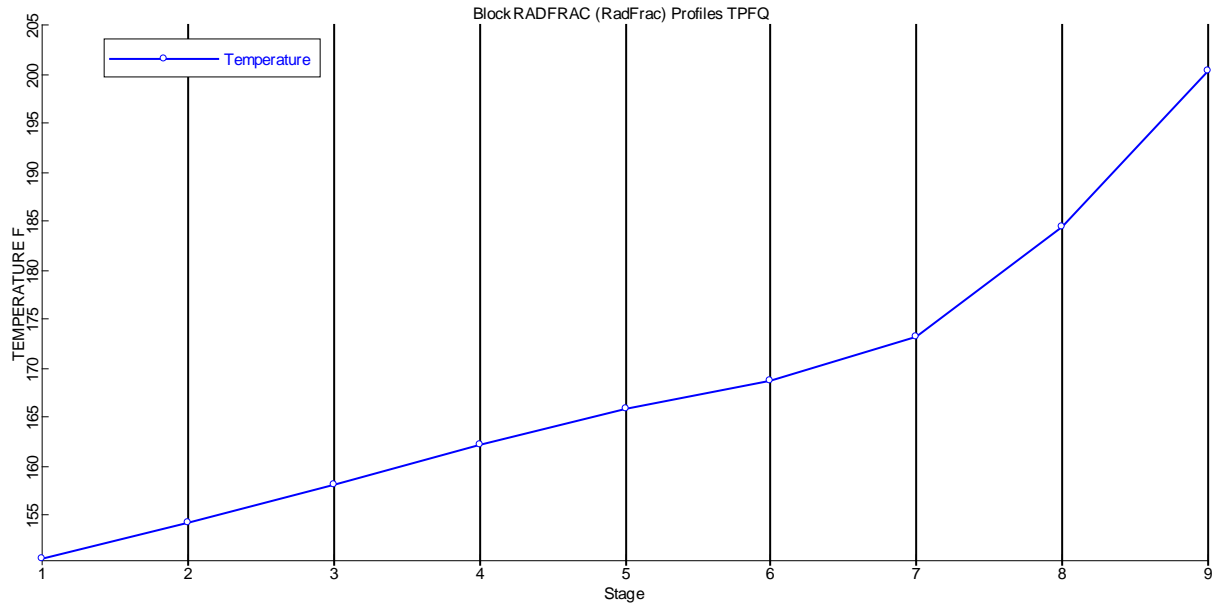
DSTWU Report with Solutions:

```
        *** RESULTS ***
DISTILLATE TEMP. (F   )              150.380
BOTTOM TEMP. (F     )           201.425
MINIMUM REFLUX RATIO                0.50445
ACTUAL REFLUX RATIO                 0.50496
MINIMUM STAGES              4.06022
ACTUAL EQUILIBRIUM STAGES             196.222
NUMBER OF ACTUAL STAGES ABOVE FEED         122.013
DIST. VS FEED              0.41110
CONDENSER COOLING REQUIRED (BTU/HR )       951,298.
NET CONDENSER DUTY (BTU/HR  )       -951,298.
REBOILER HEATING REQUIRED (BTU/HR )        989,262.
NET REBOILER DUTY (BTU/HR  )        989,262.
```

RadFrac Report with Solutions:

```
 ***   SUMMARY OF KEY RESULTS   ***

TOP STAGE TEMPERATURE       F            150.557
BOTTOM STAGE TEMPERATURE     F           200.382
TOP STAGE LIQUID FLOW      LBMOL/HR        31.0995
BOTTOM STAGE LIQUID FLOW     LBMOL/HR       58.9000
TOP STAGE VAPOR FLOW      LBMOL/HR       0.0
BOTTOM STAGE VAPOR FLOW     LBMOL/HR        64.9746
MOLAR REFLUX RATIO               0.75668
MOLAR BOILUP RATIO               1.10313
CONDENSER DUTY (W/O SUBCOOL)  BTU/HR     -1,114,320.
REBOILER DUTY          BTU/HR      1,150,940.
```

Notes: