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.

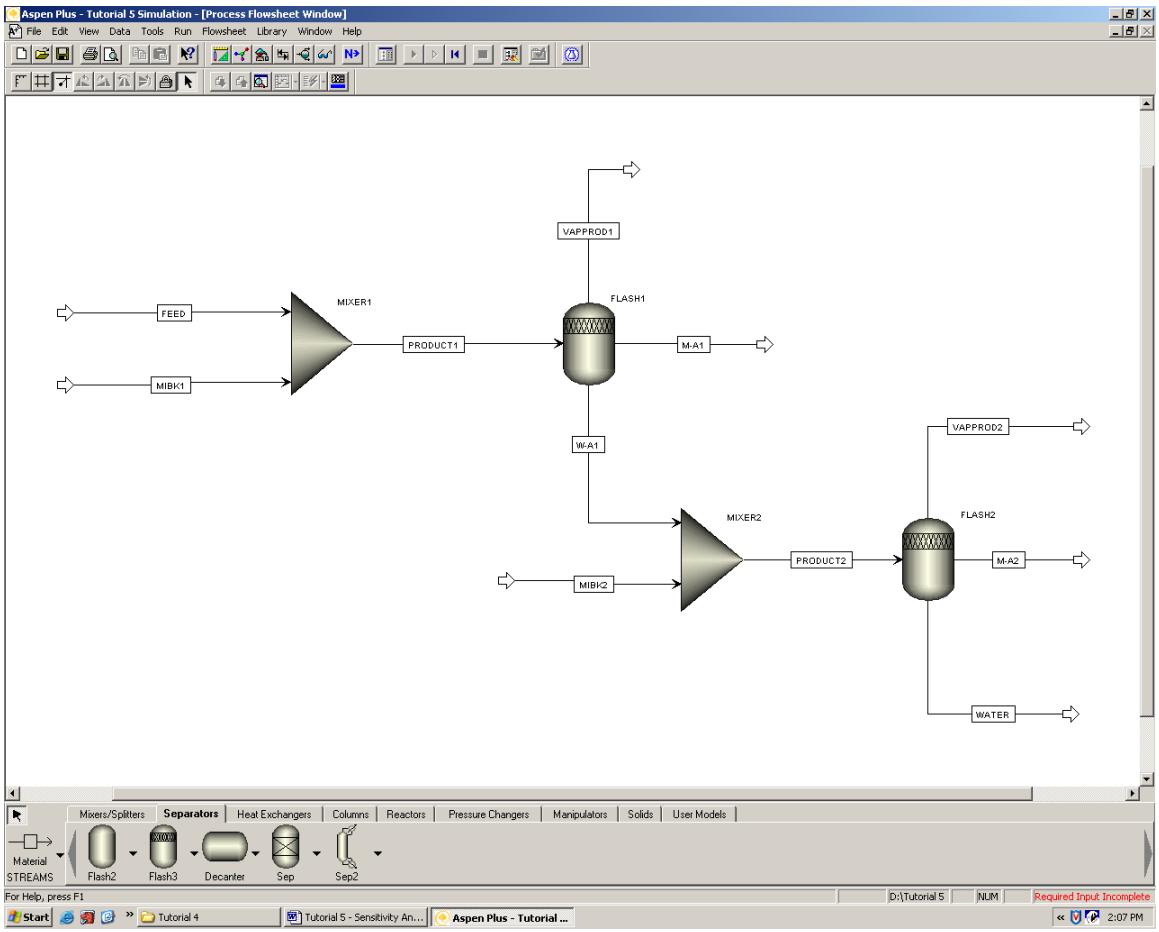

Figure 1: Updated Process Flowsheet

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).

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.

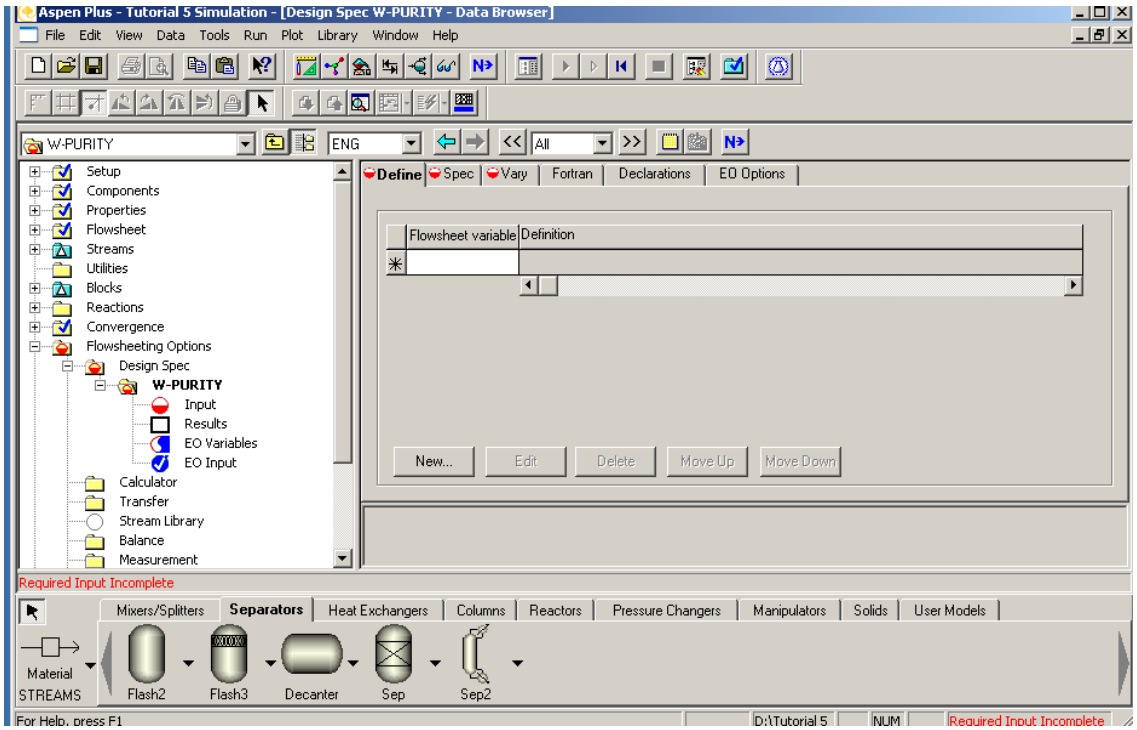

Figure 3: Design Specification Window

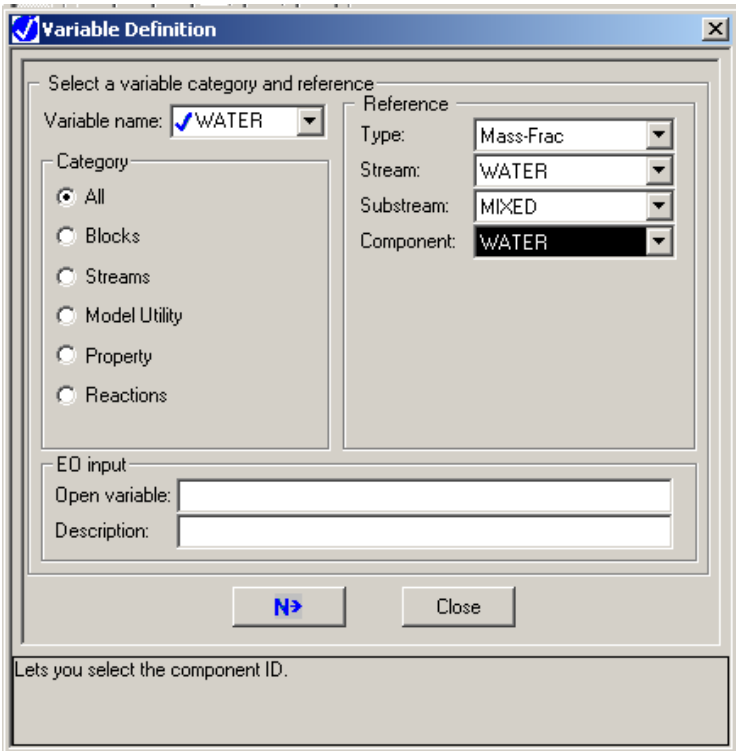

Figure 4: Completed Variable Definition Window

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.

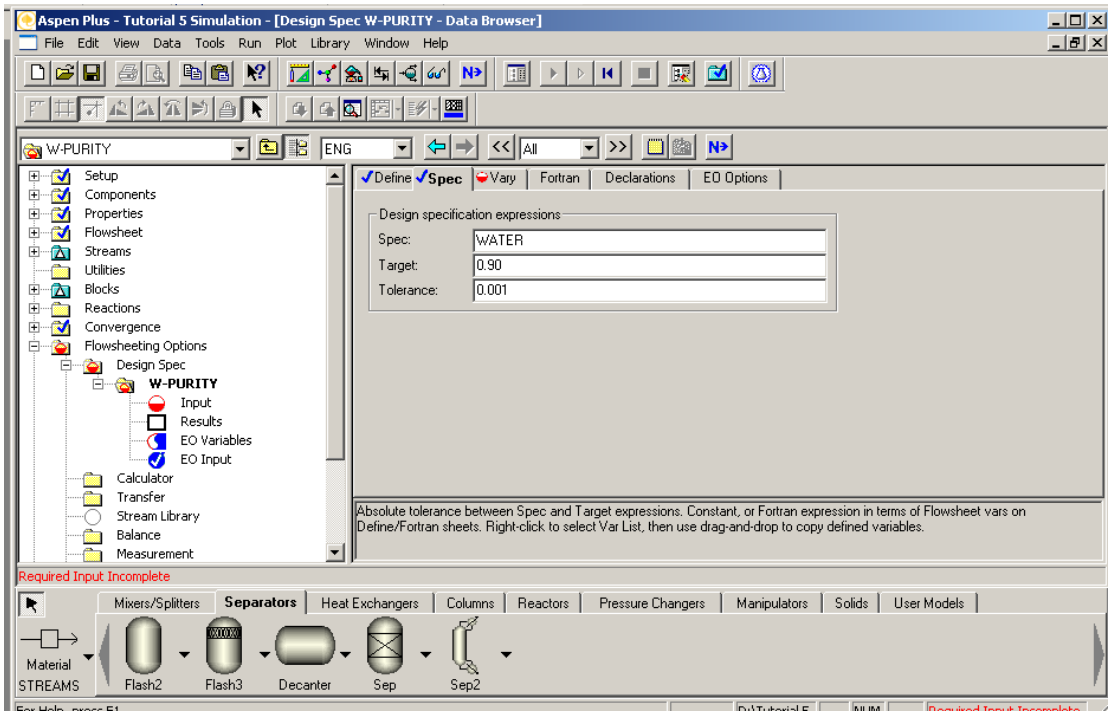

Figure 5: Completed Spec Window

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.

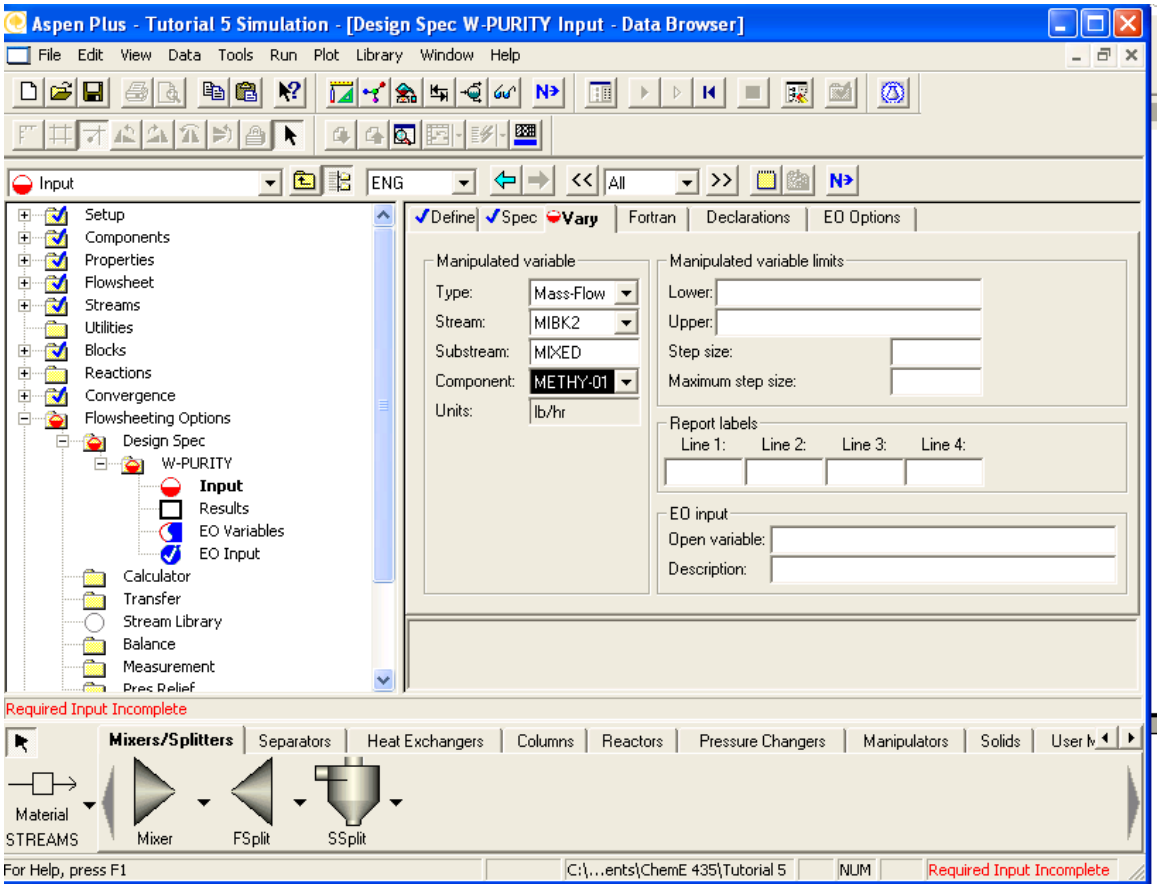

Figure 6: Vary Tab Options

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.

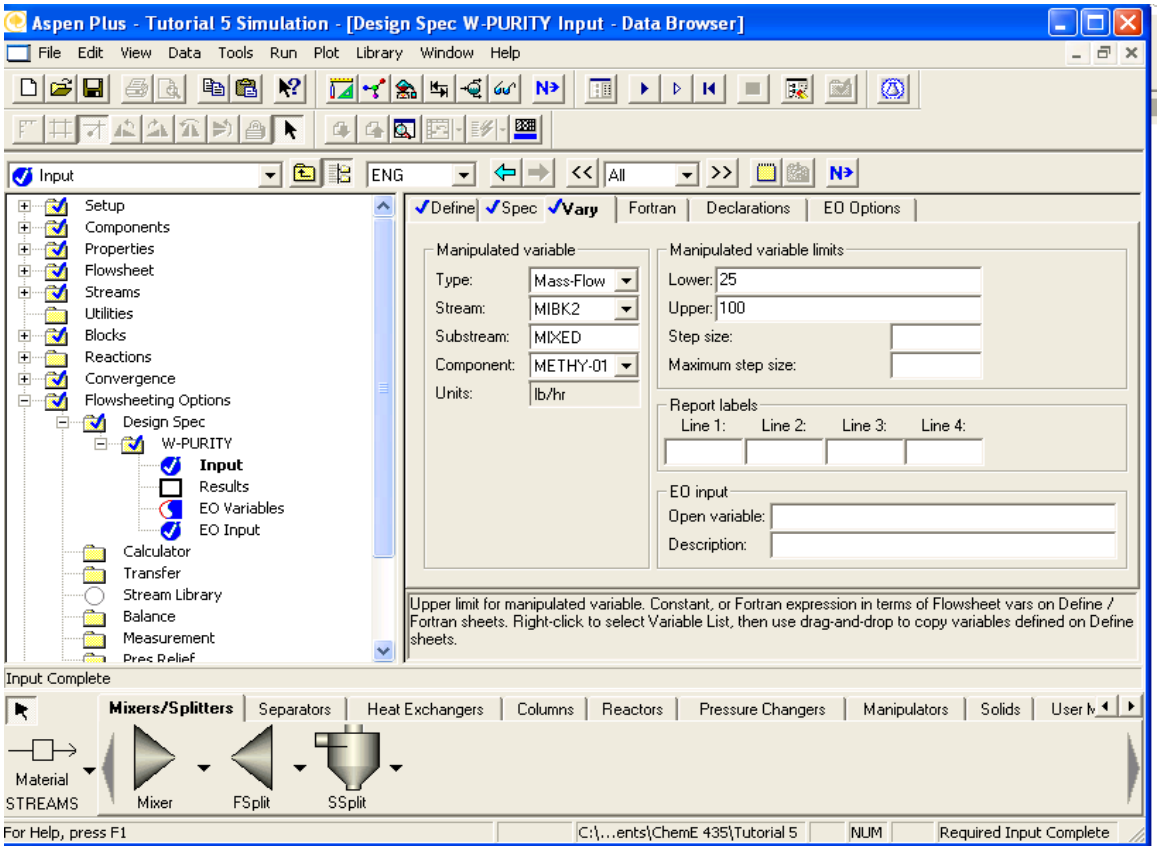

Figure 7: Completed Vary Window

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.

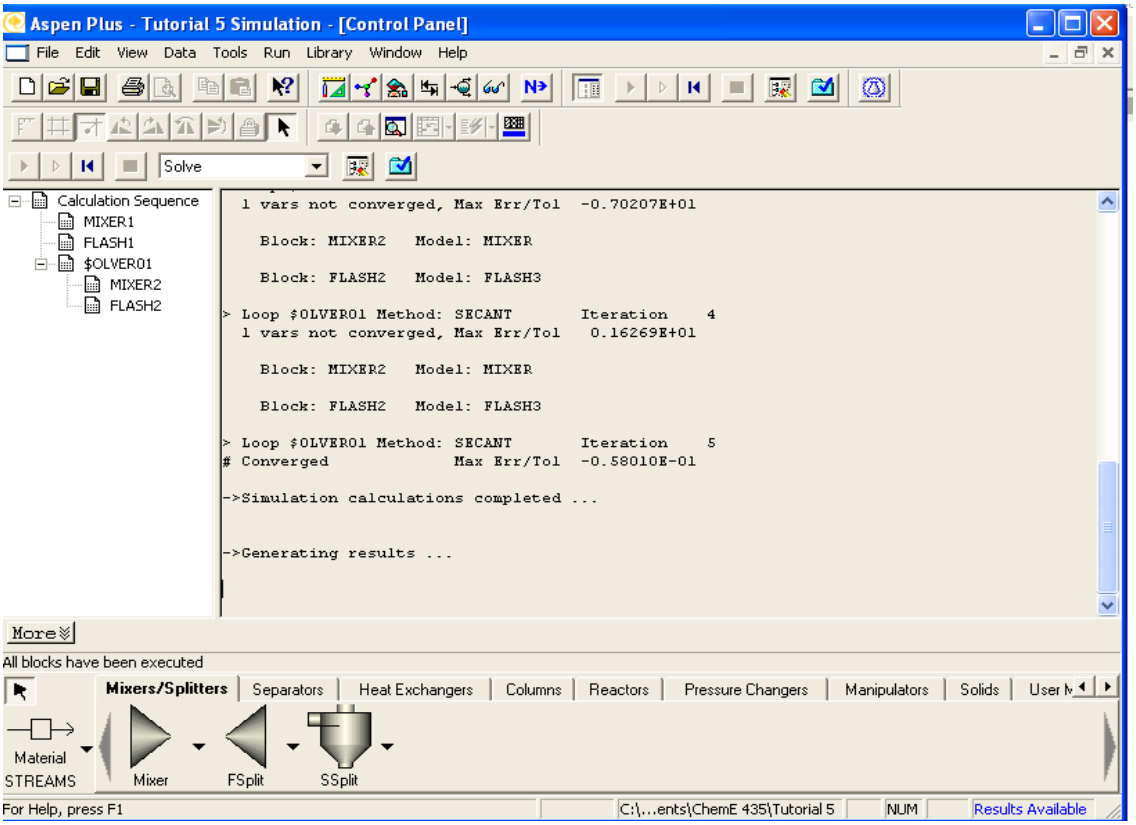

Figure 8: Run Control Panel

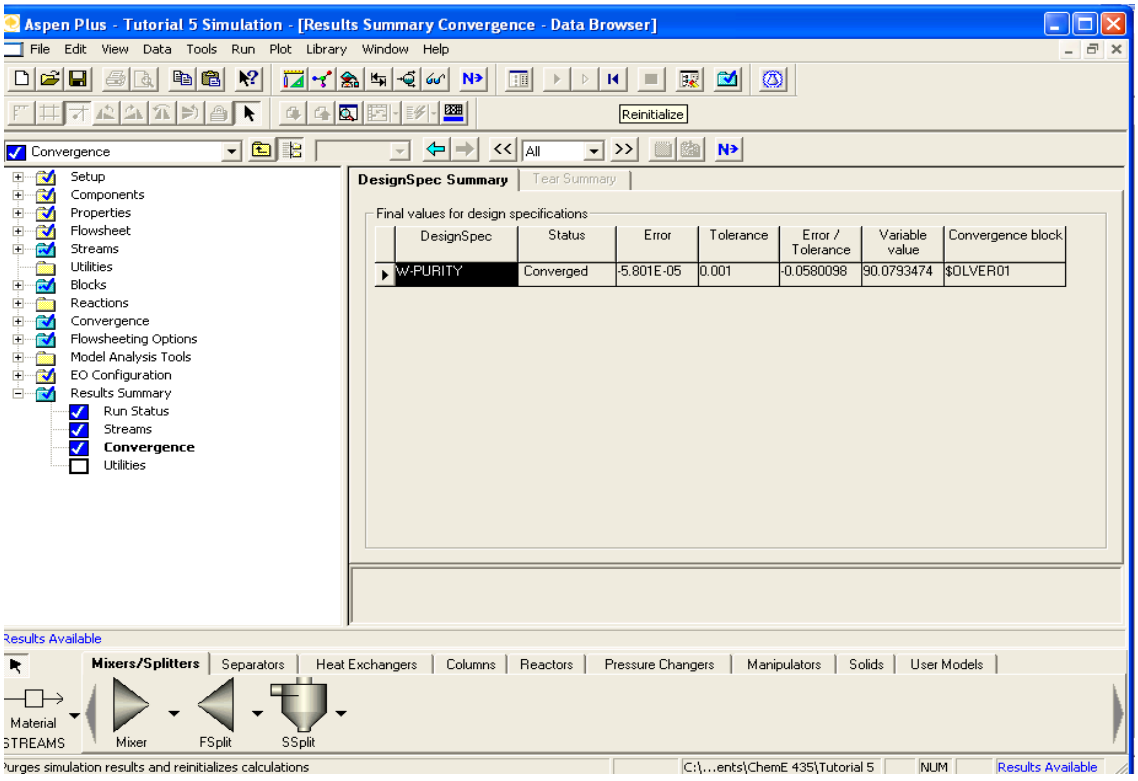

Figure 9: Convergence Results

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

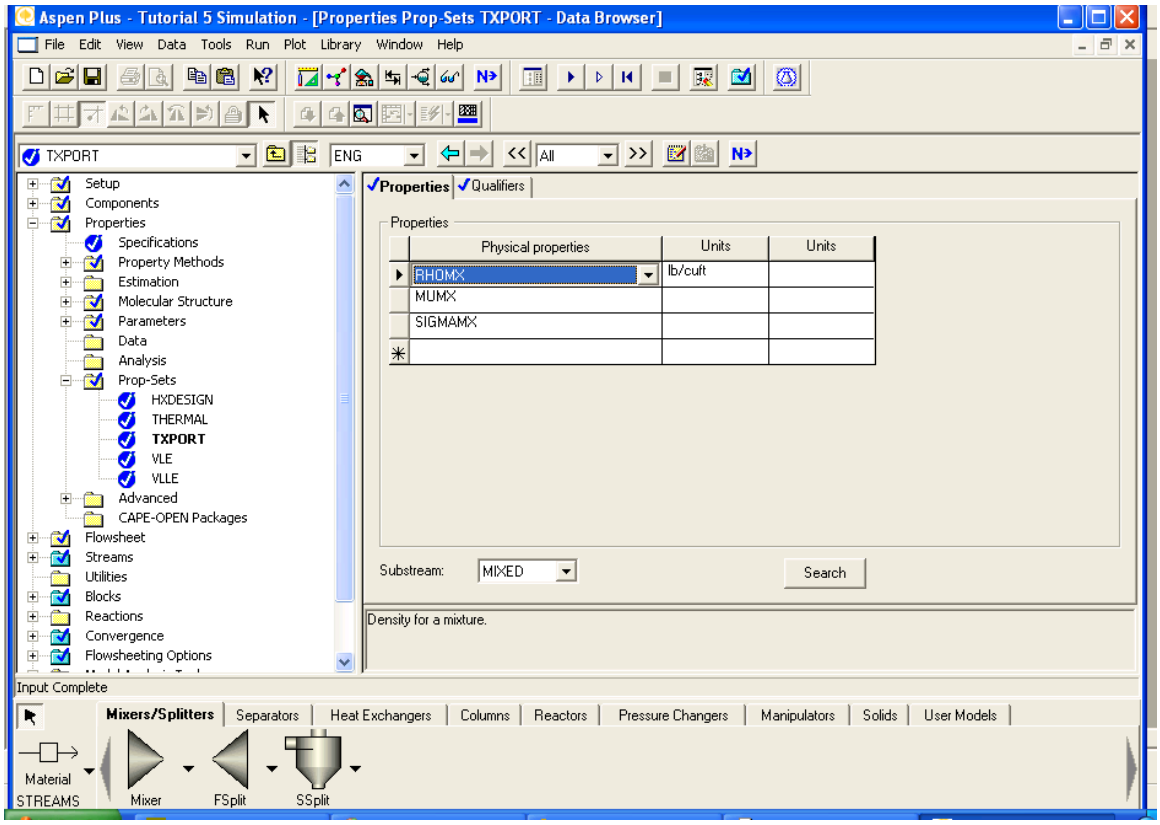

Figure 10: TXPORT Edit Window

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.

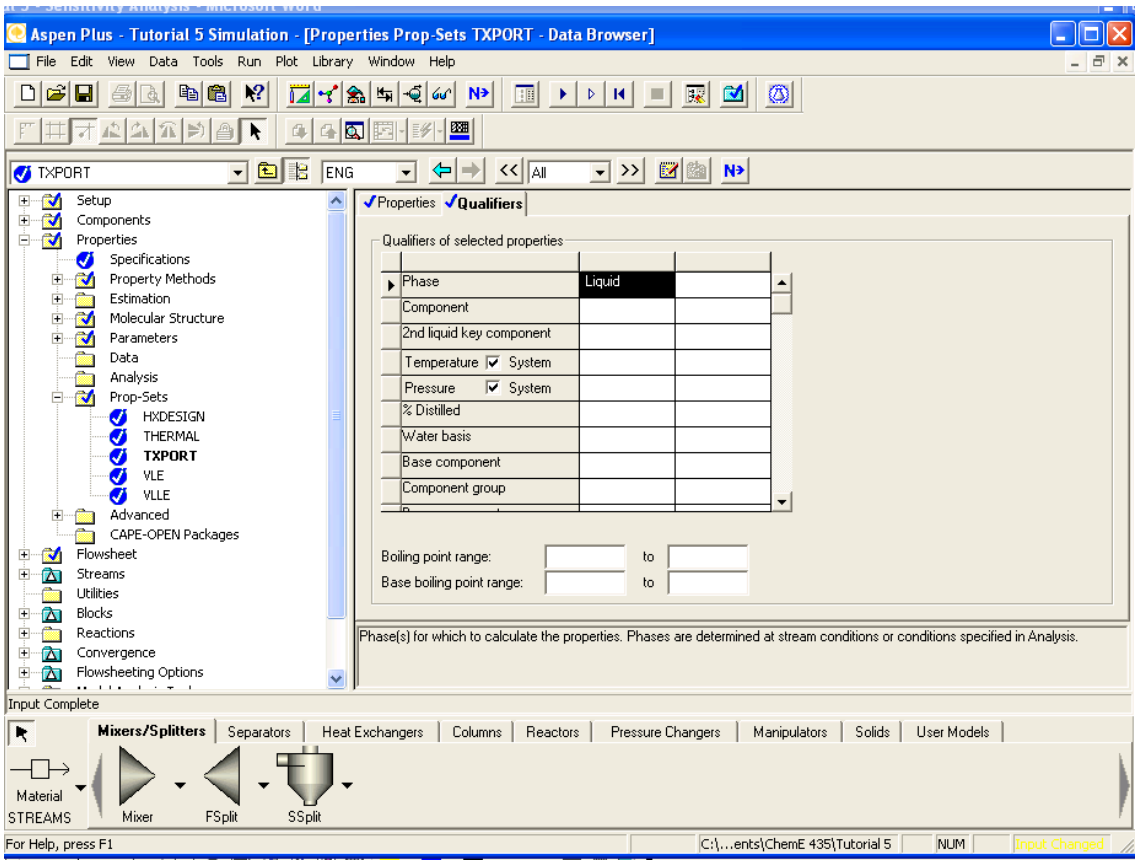

Figure 11: Qualifiers Window

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.

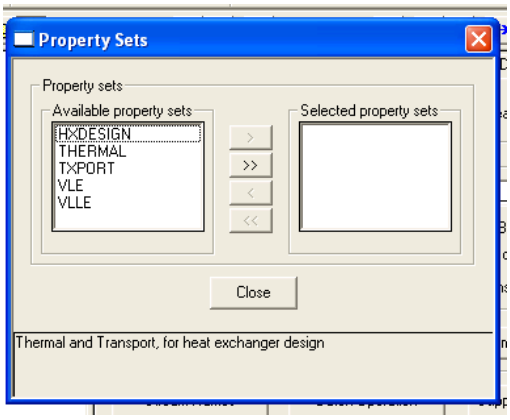

Figure 12: Property Sets Window

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
VolumeFlow	cuft/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
*** LIQUIDPHASE ***								
Density	lb/cuft	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
SurfaceTen	dyne/cm	61.235	23.538	23.538	31.578	29.101	68.595	71.528
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

Figure 13: Final Stream Table

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

Tutorial #5 Homework

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!

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.

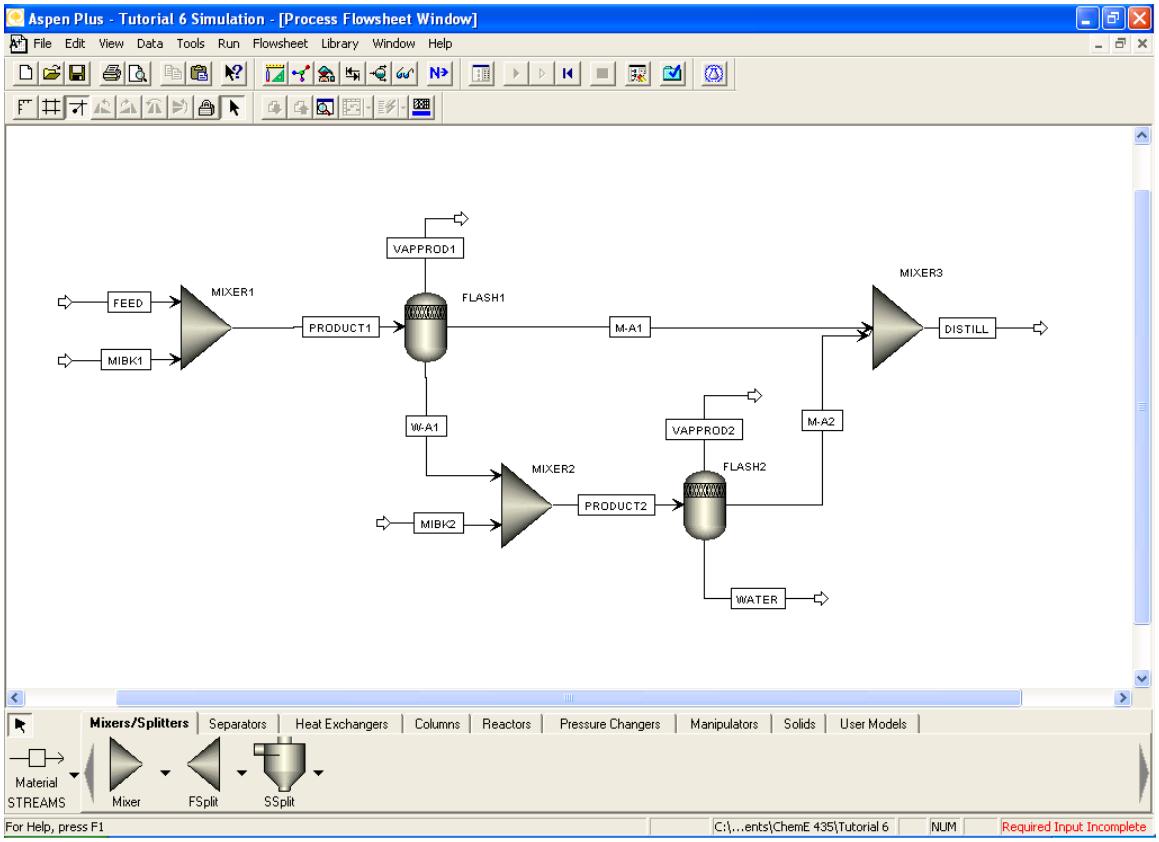

Figure 1: Acetone/MIBK Mixer

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.

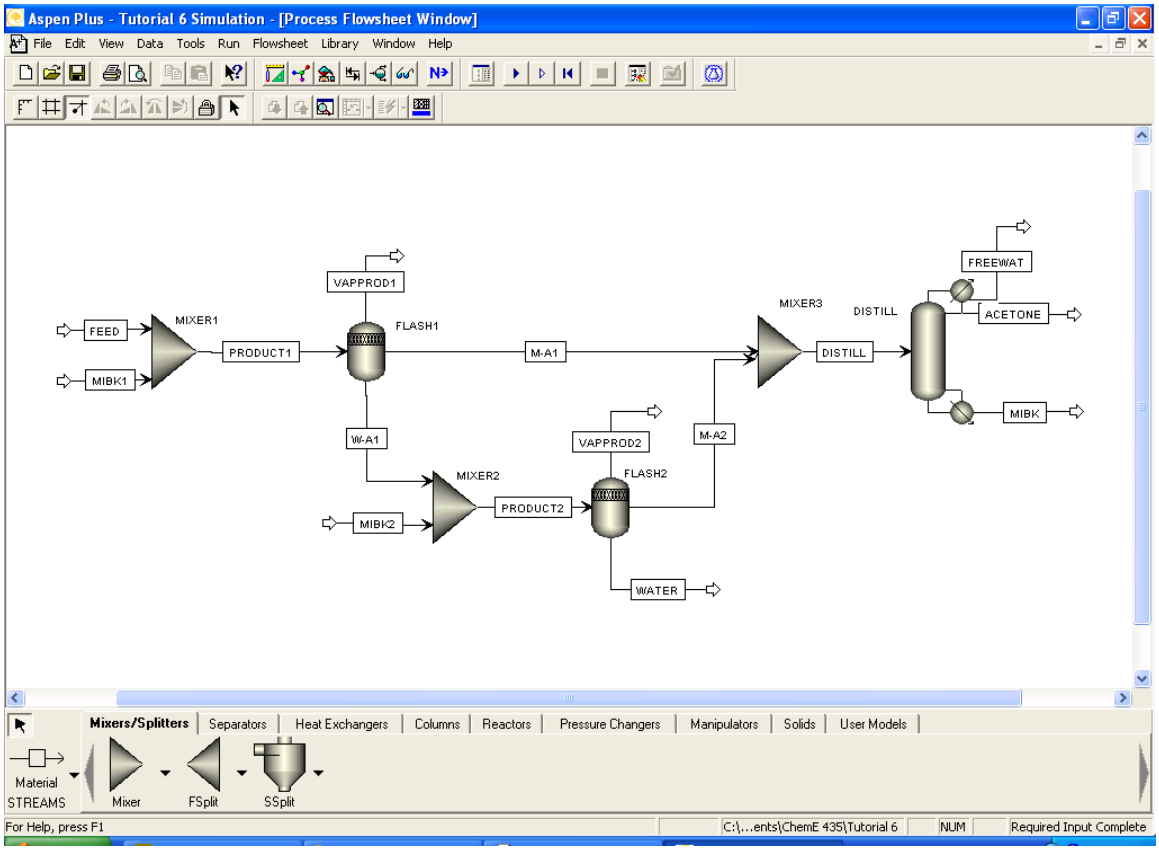

Figure 2: Completed Process Flowsheet

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.

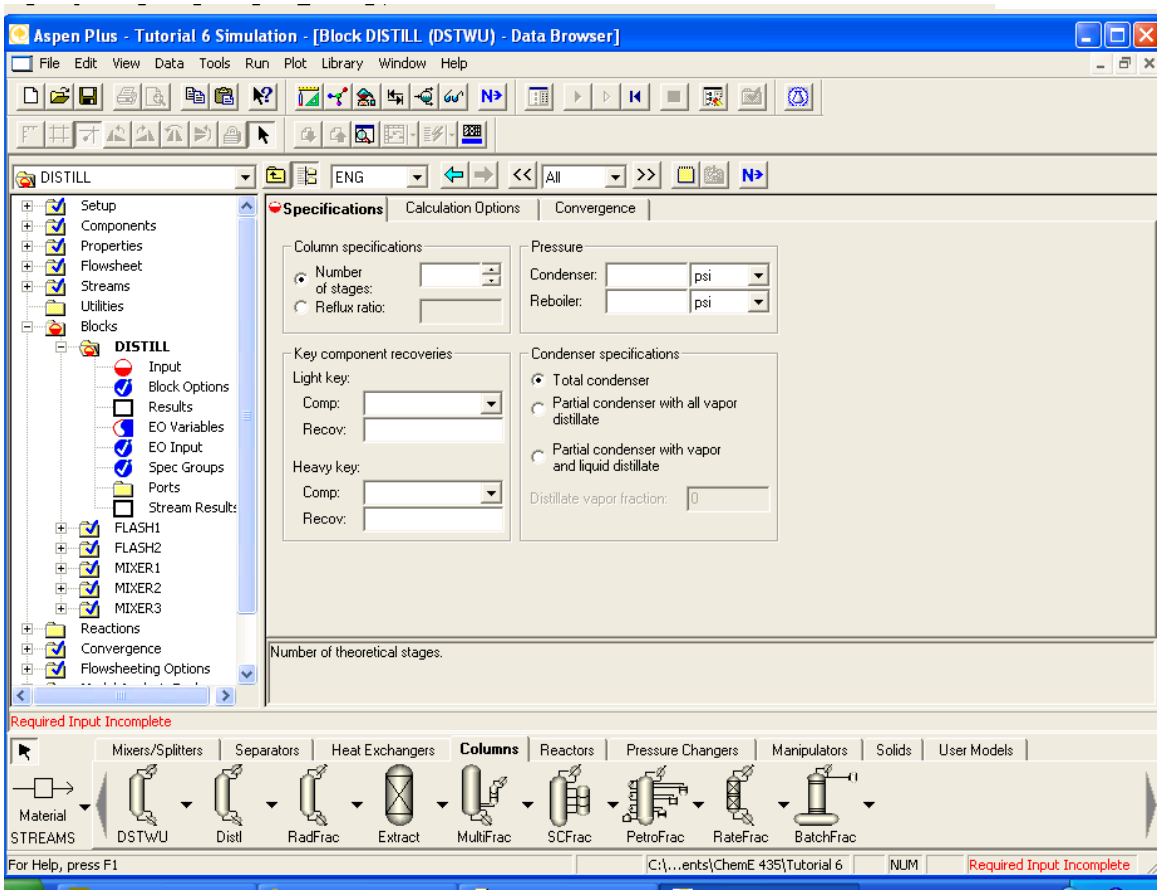

Figure 3: DSTWU Data Input Window

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.

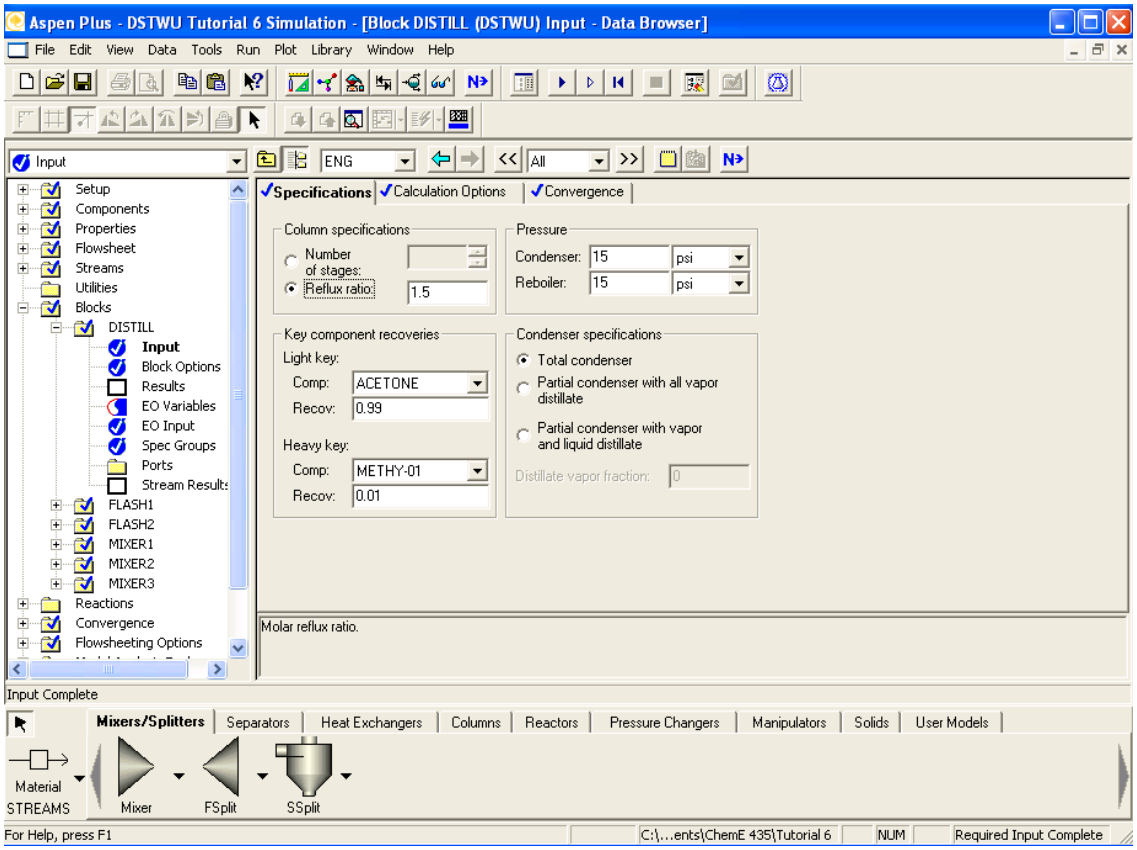

Figure 4: Completed DSTWU Input Window

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.

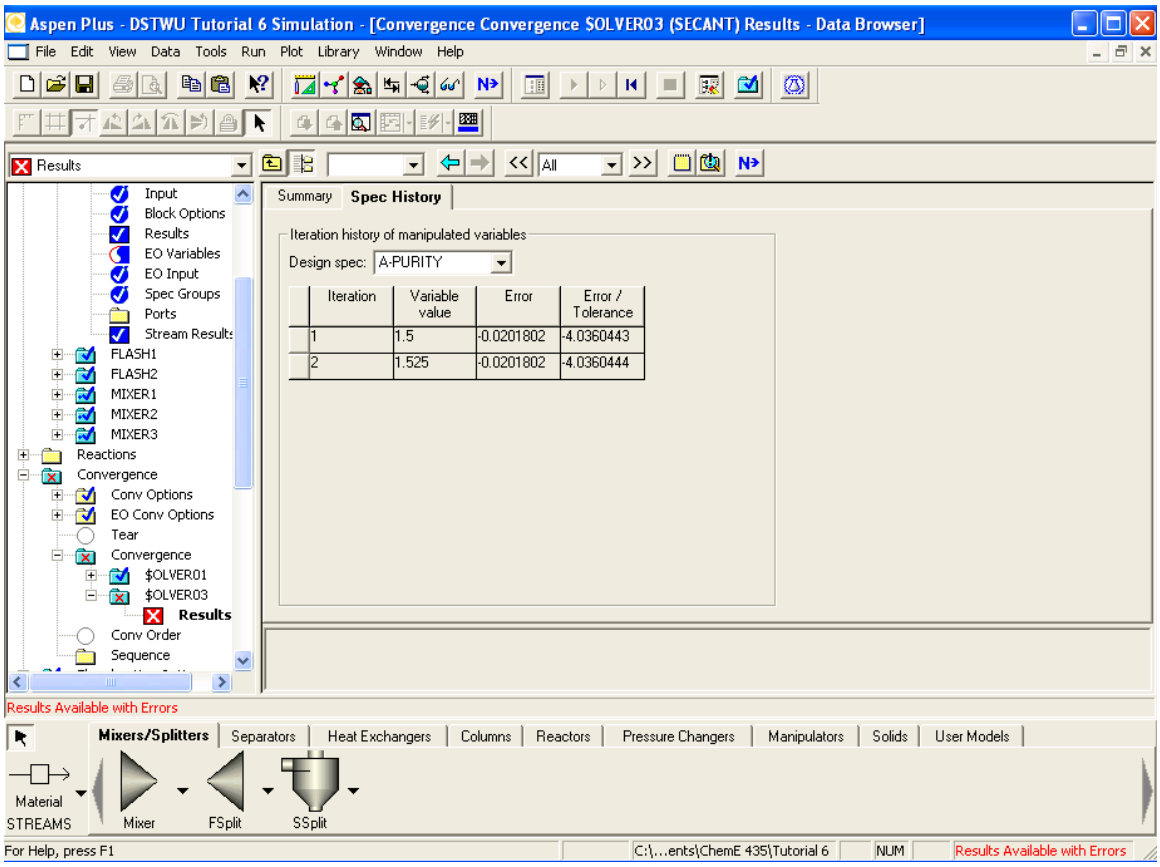

Figure 6: Convergence Window

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.

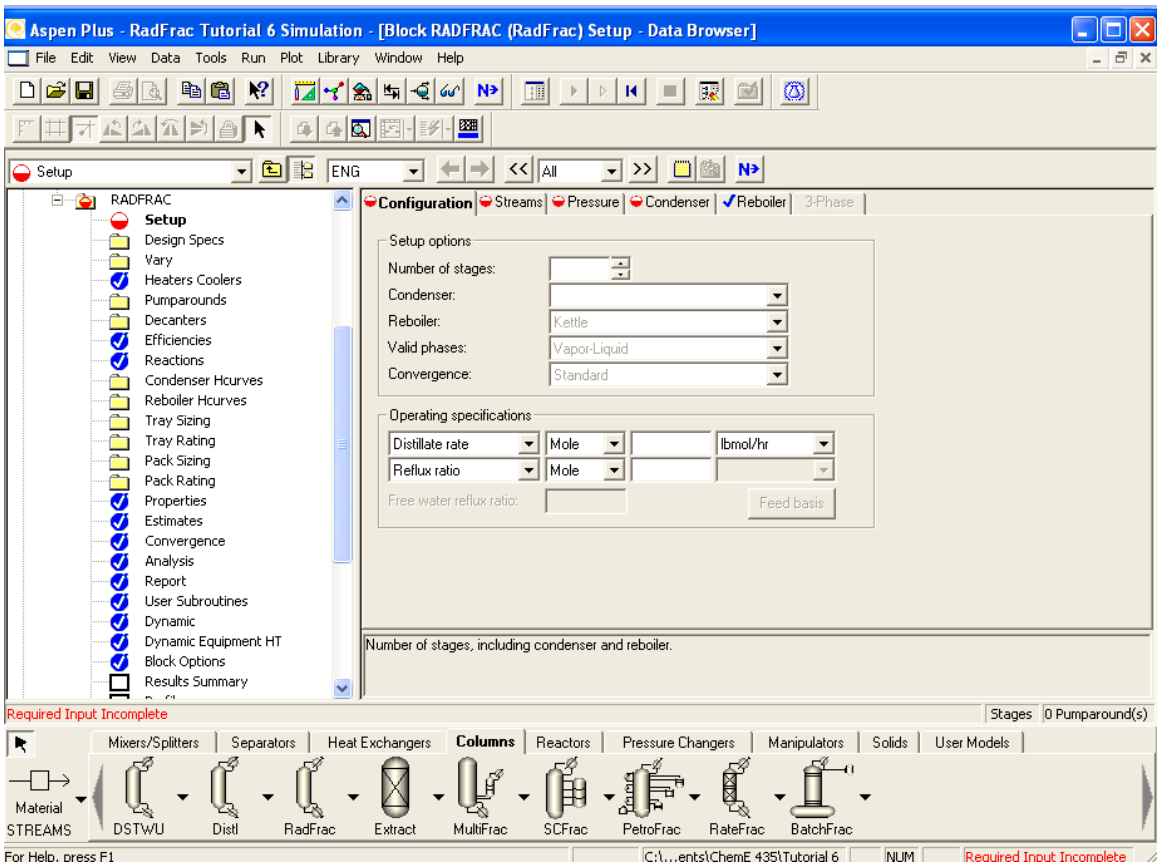

Figure 7: RadFrac Input Window

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.

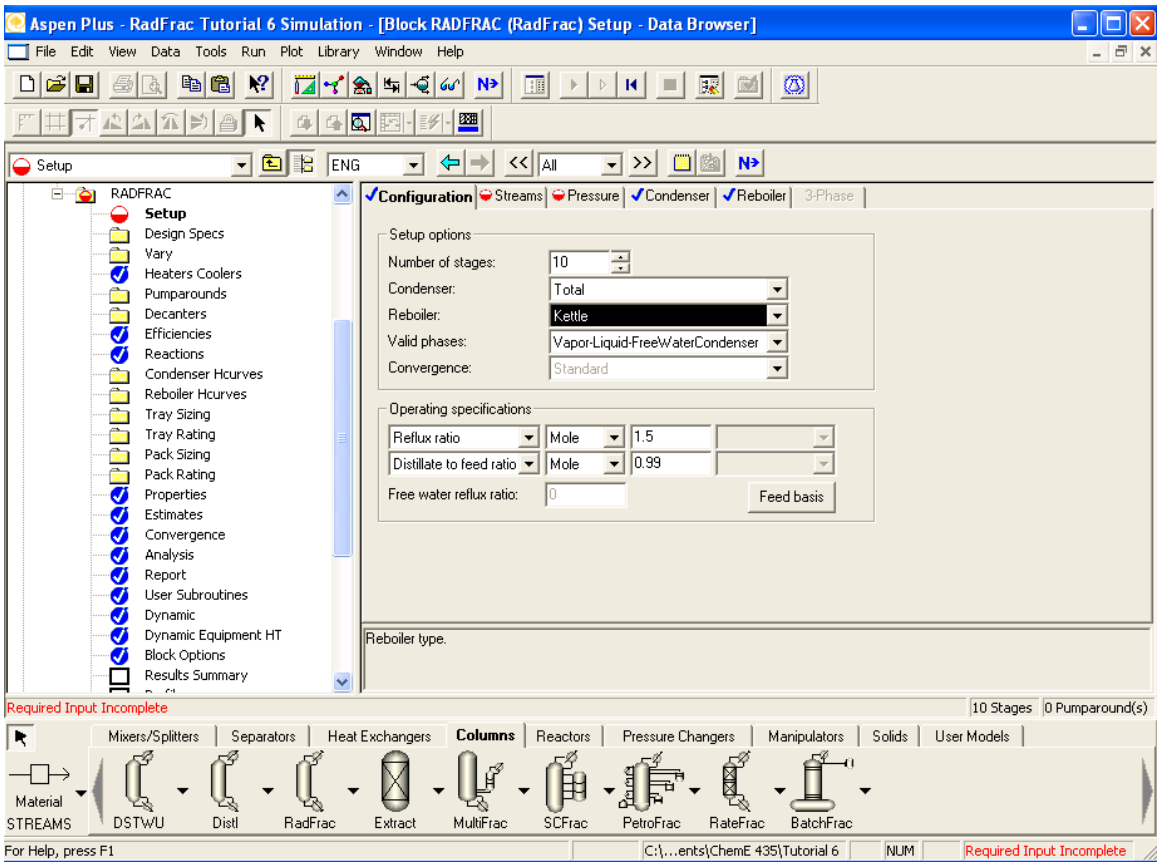

Figure 8: Completed Configuration Input

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

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.

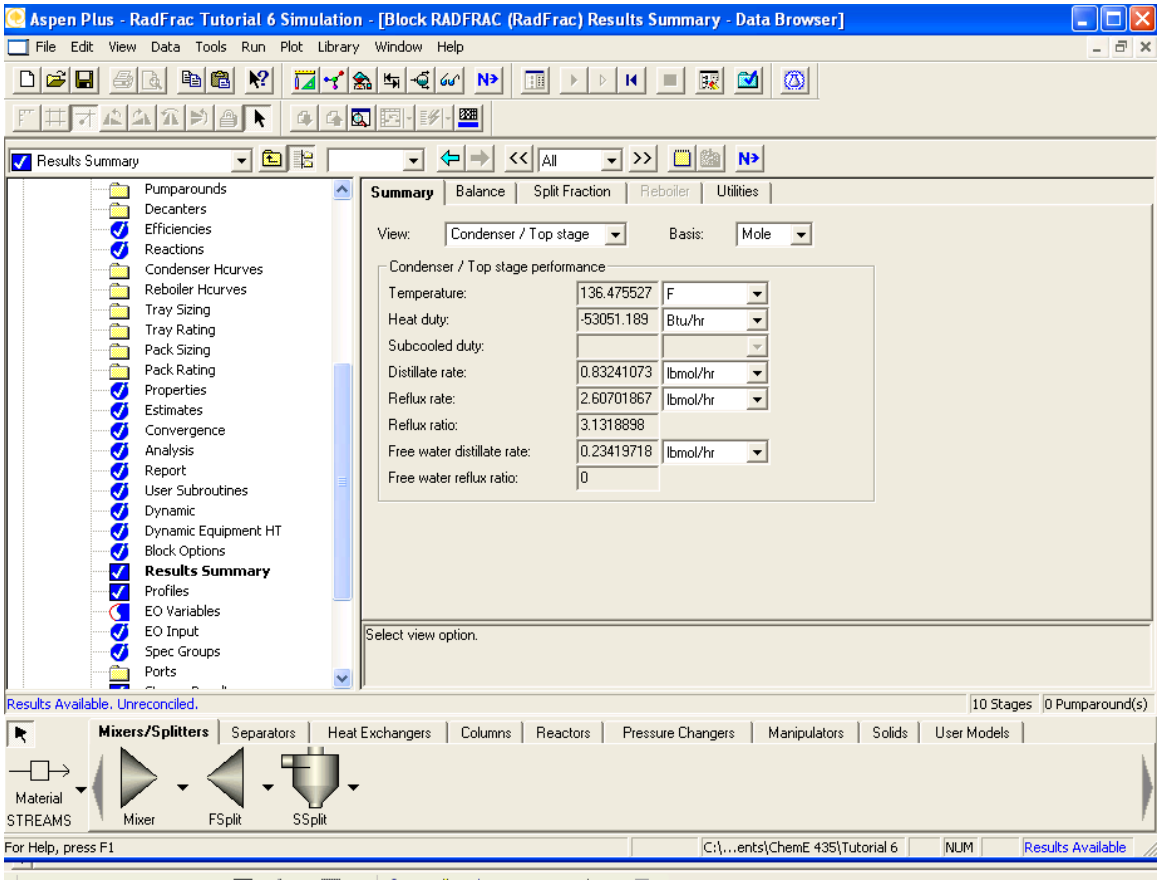

Figure 11: RadFrac Results Summary

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

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.

Final Homework

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).