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.

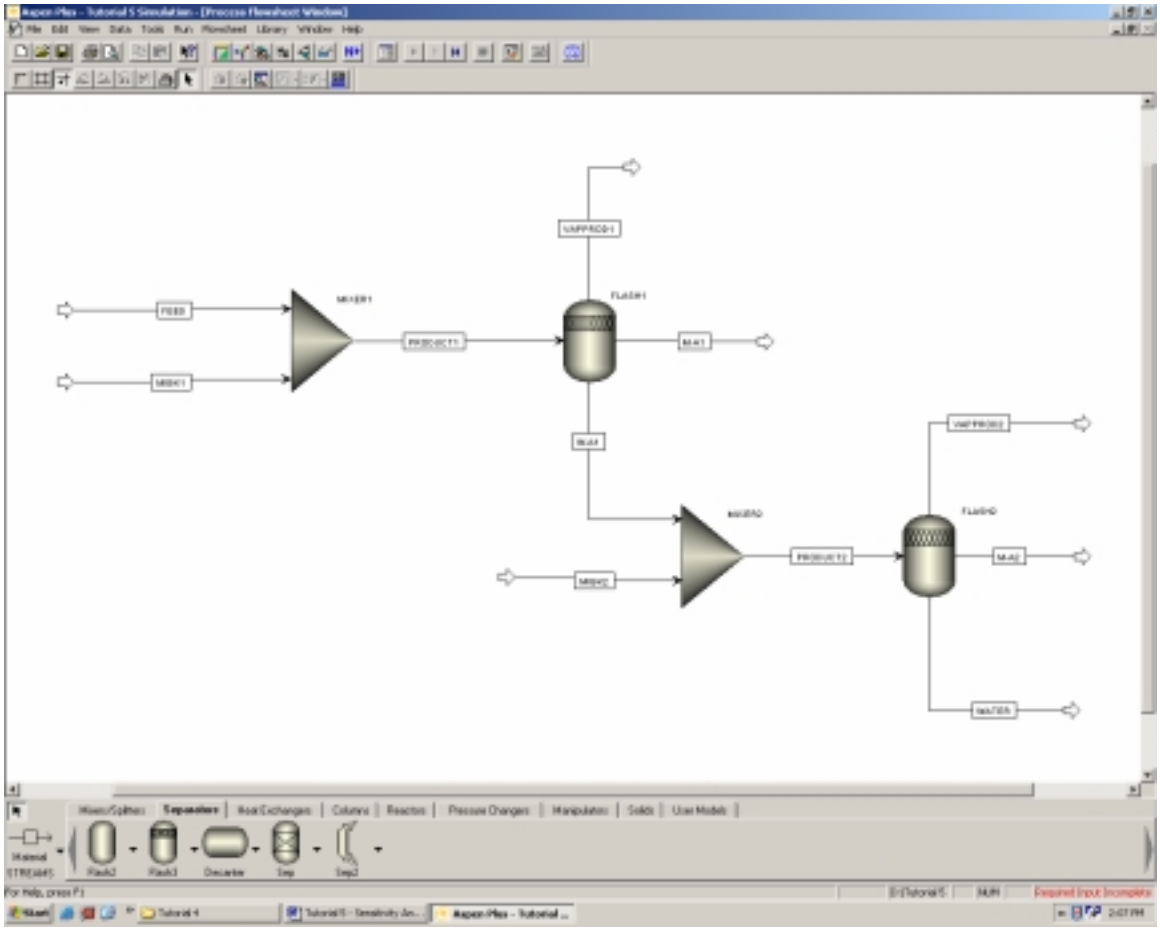

Figure 1: Updated Process Flowsheet

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.

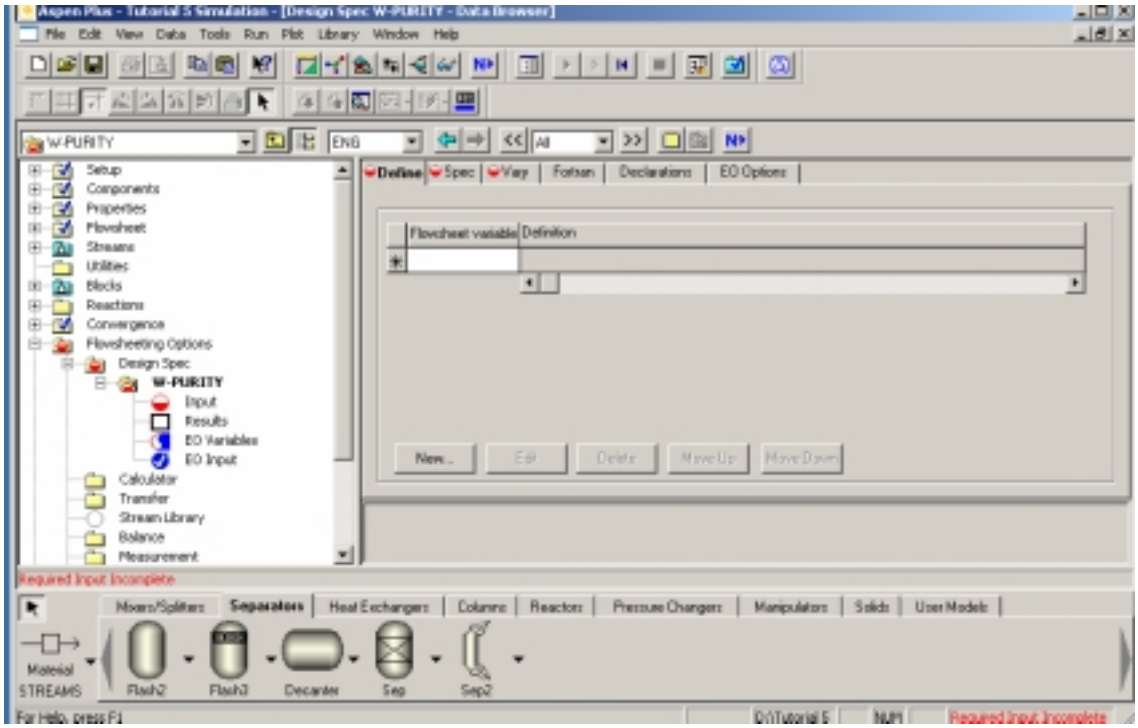

Figure 3: Design Specification Window

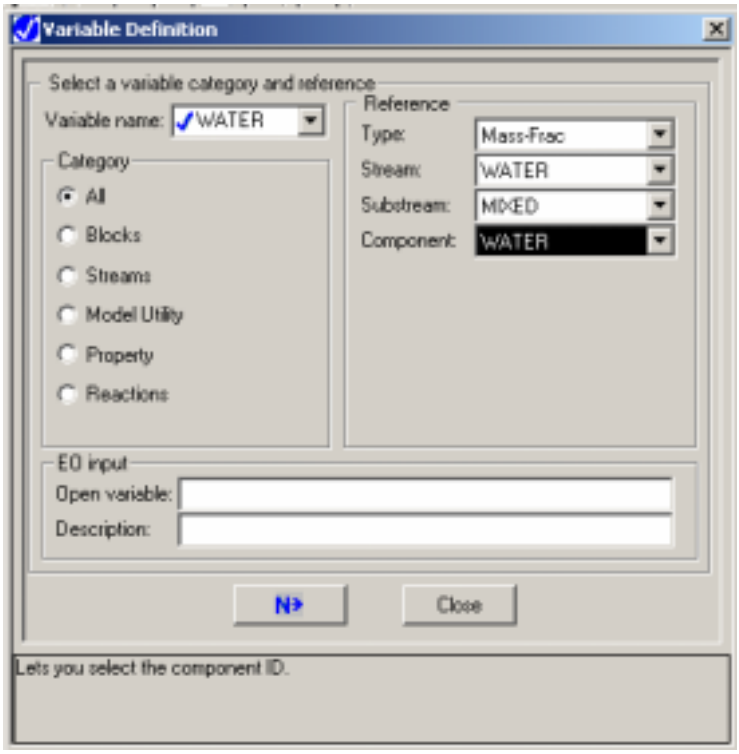

Figure 4: Completed Variable Definition Window

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.

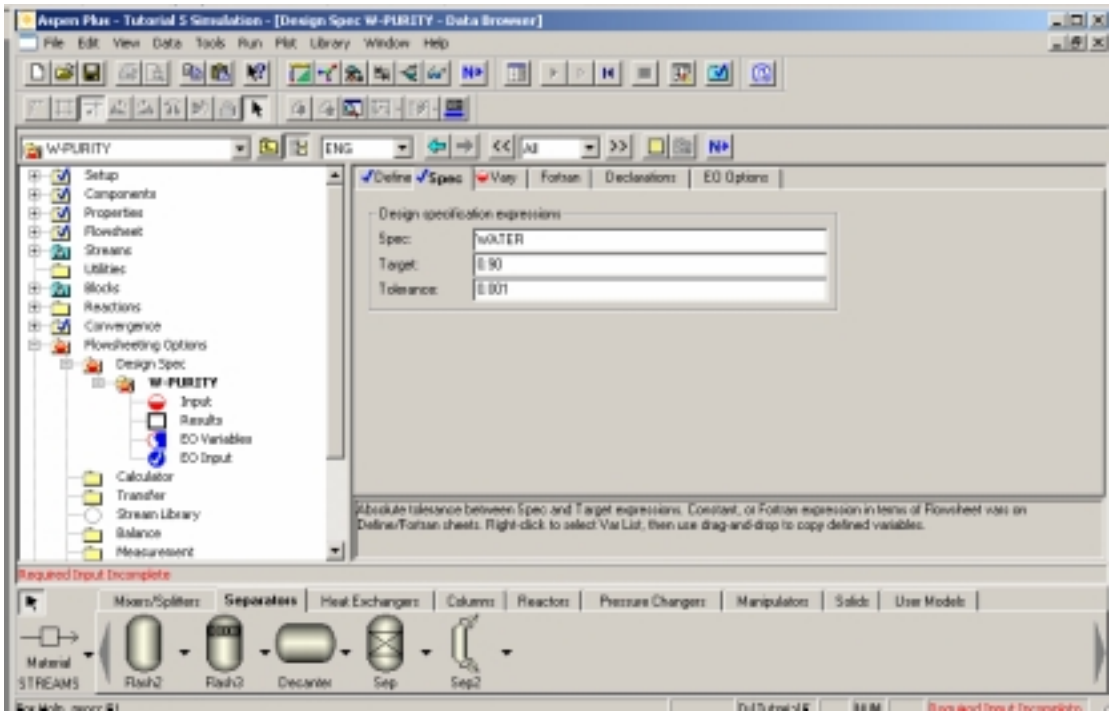

Figure 5: Completed Spec Window

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.

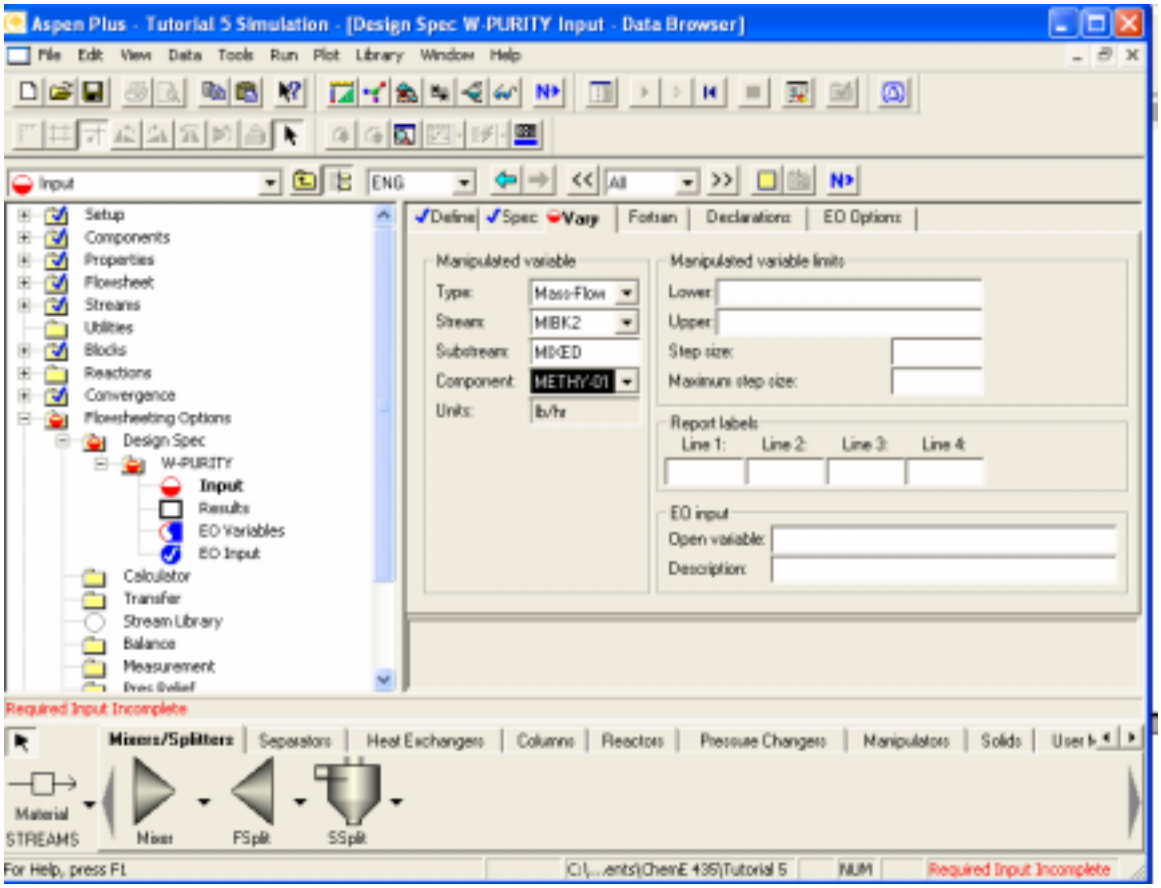

Figure 6: Vary Tab Options

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.

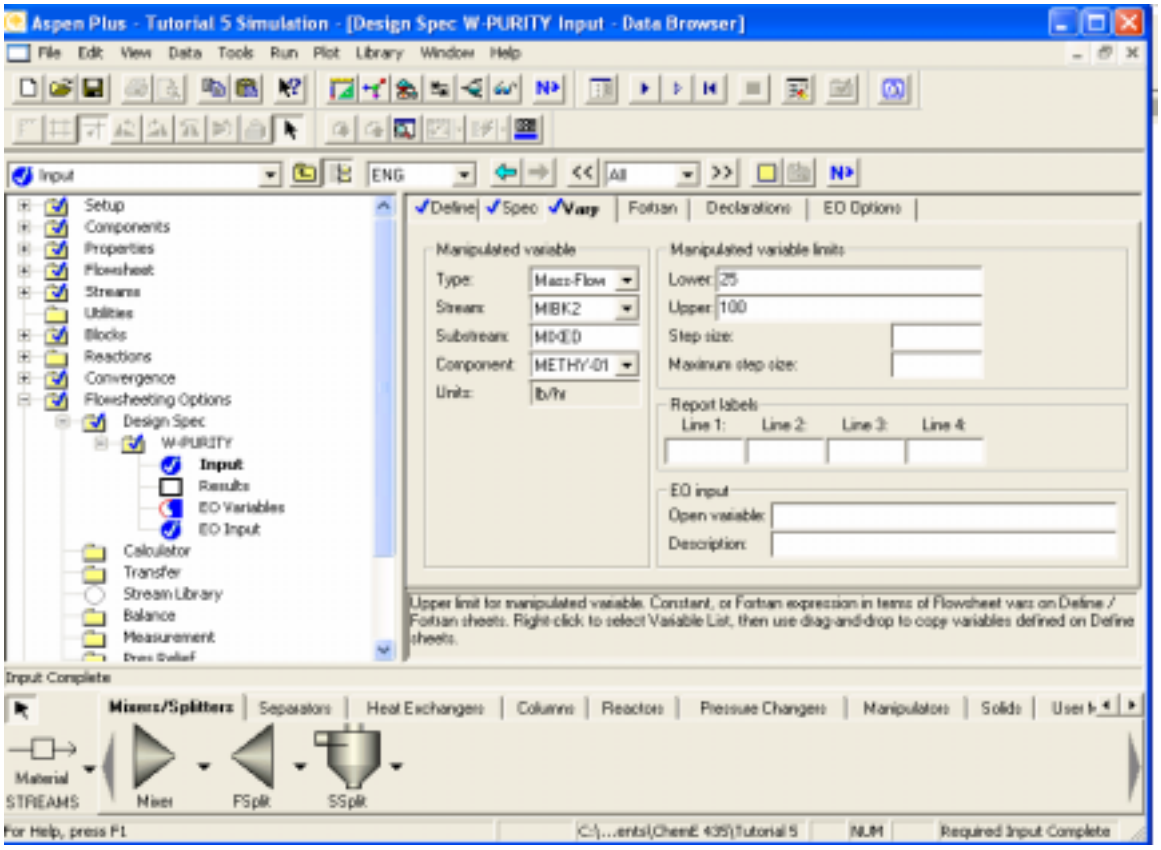

Figure 7: Completed Vary Window

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.

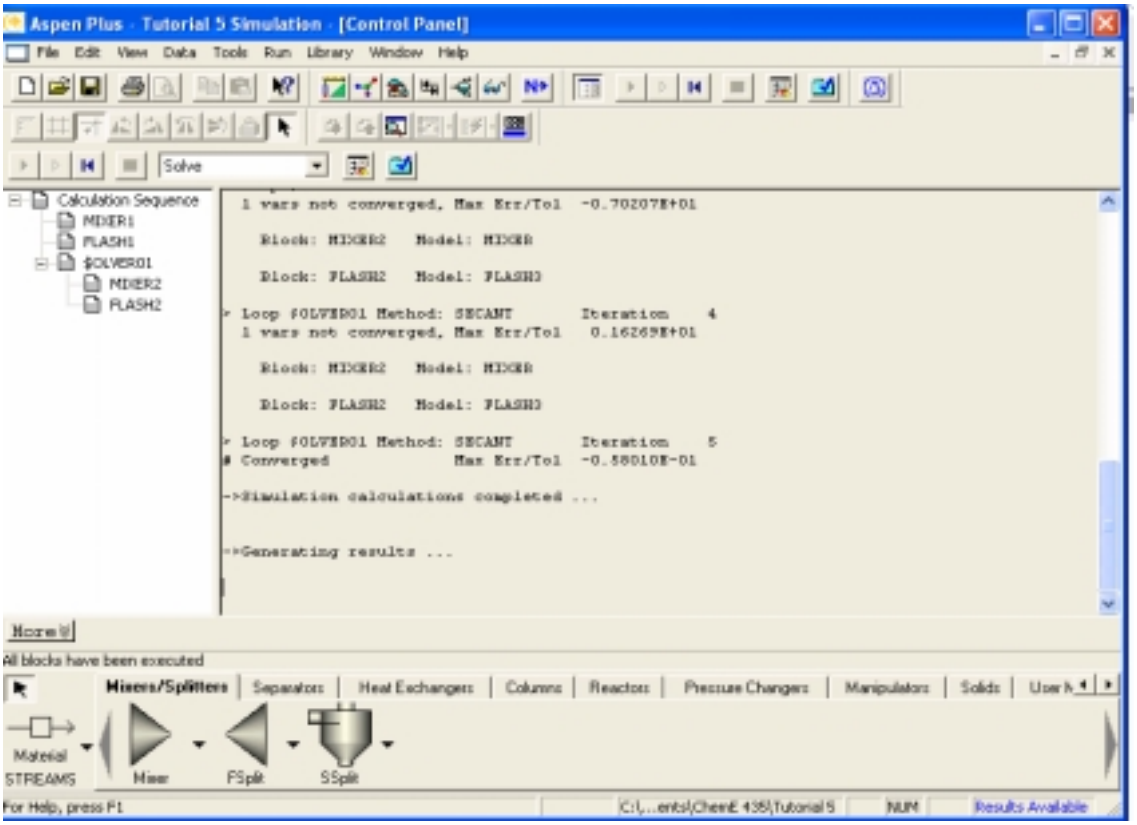

Figure 8: Run Control Panel

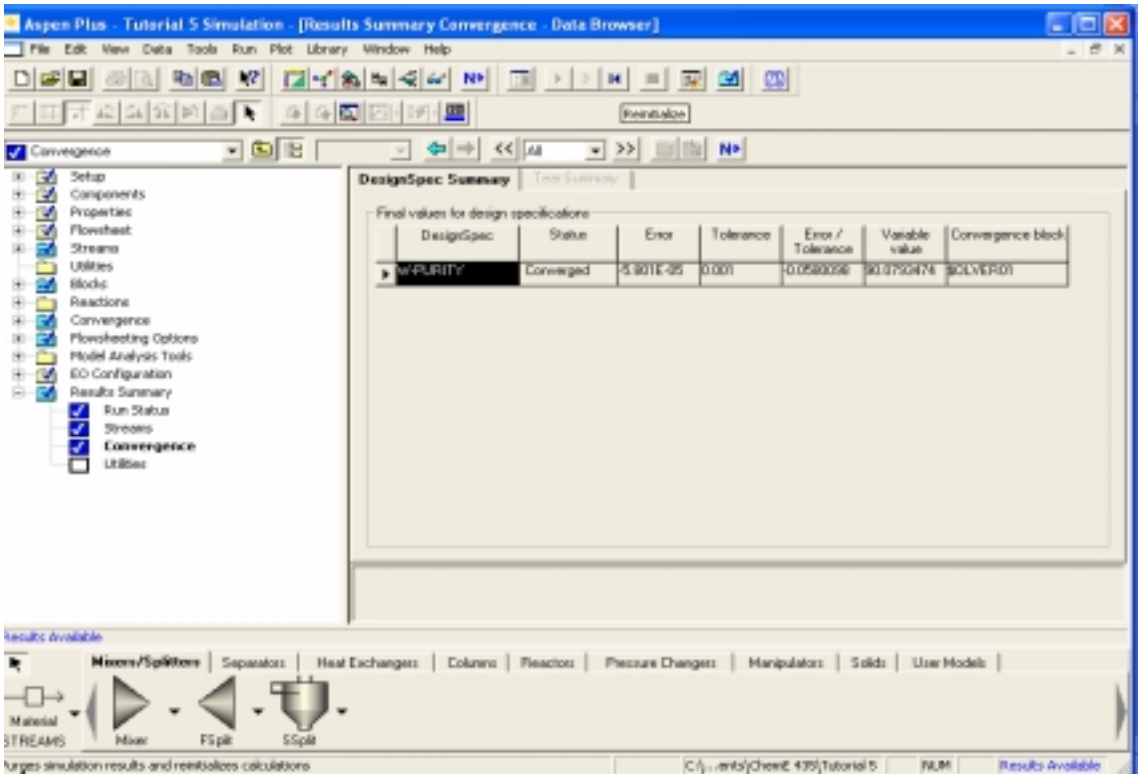

Figure 9: Convergence Results

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

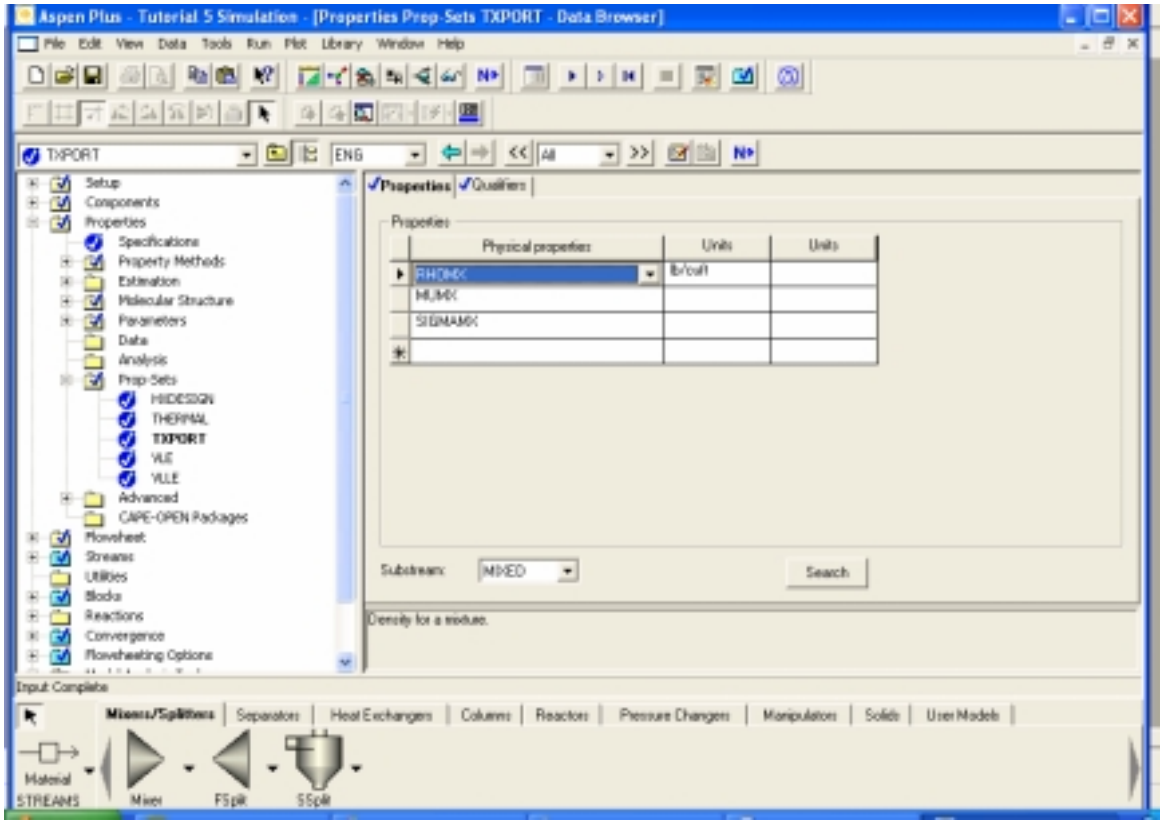

Figure 10: TXPORT Edit Window

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.

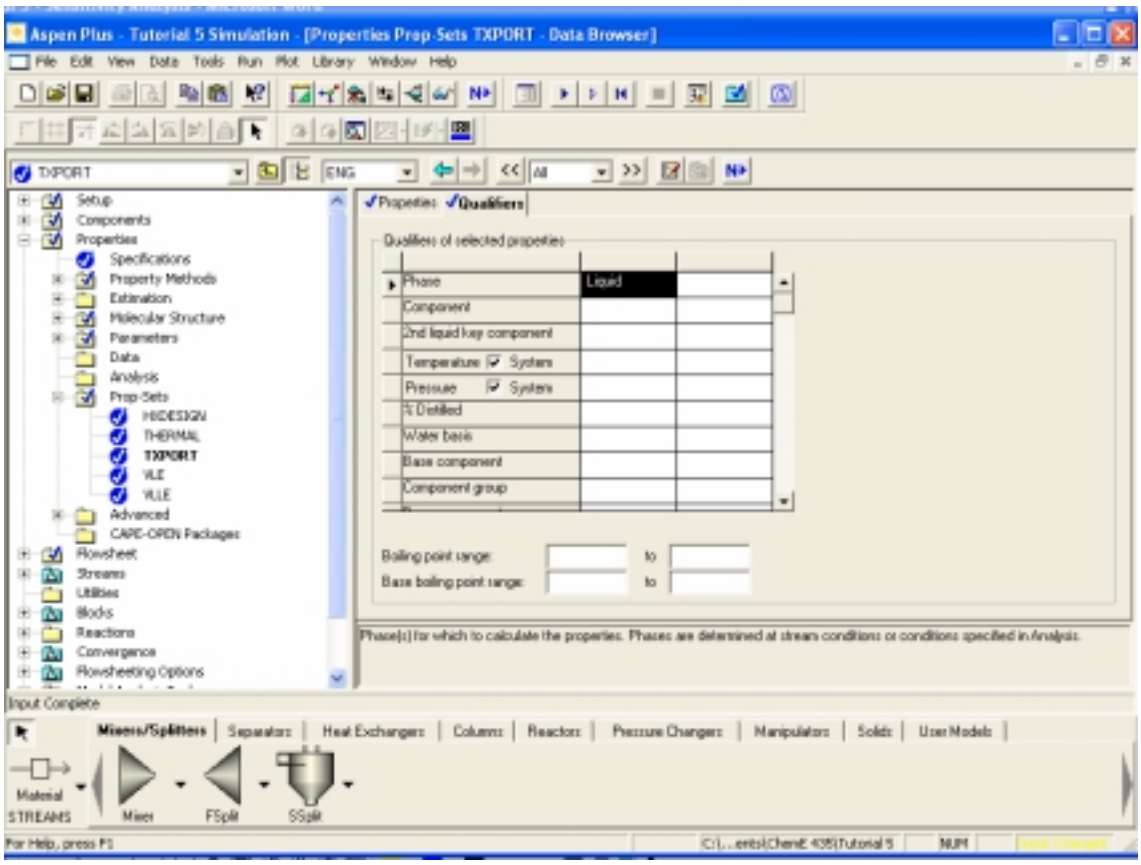

Figure 11: Qualifiers Window

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.

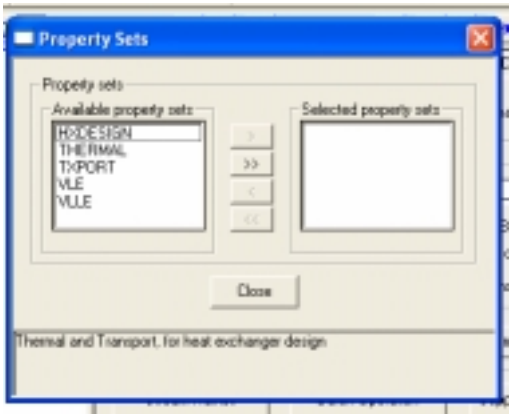

Figure 12: Property Sets Window

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.

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	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	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
*** LIQUID PHASE ***								
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 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