Aspen Tutorial #3: Flash Separation

Outline:

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- 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.
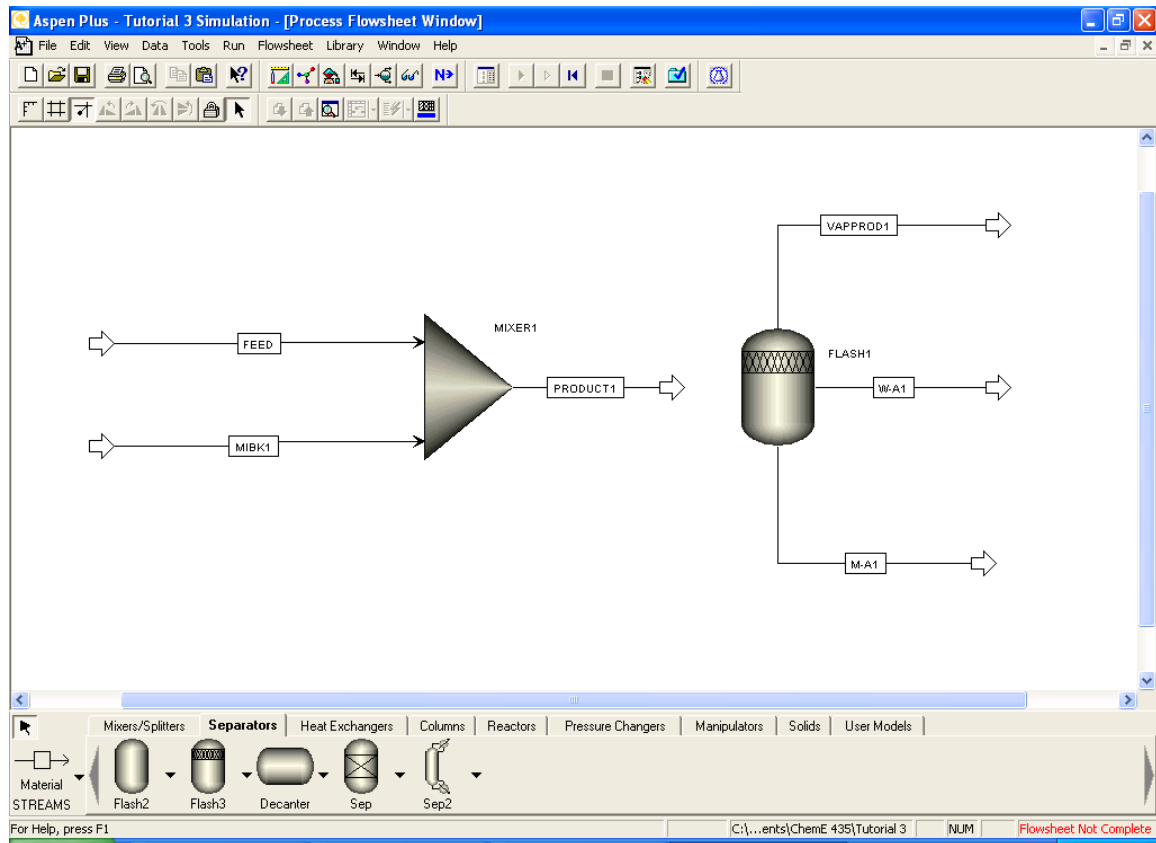
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Figure 1: Flash Separator

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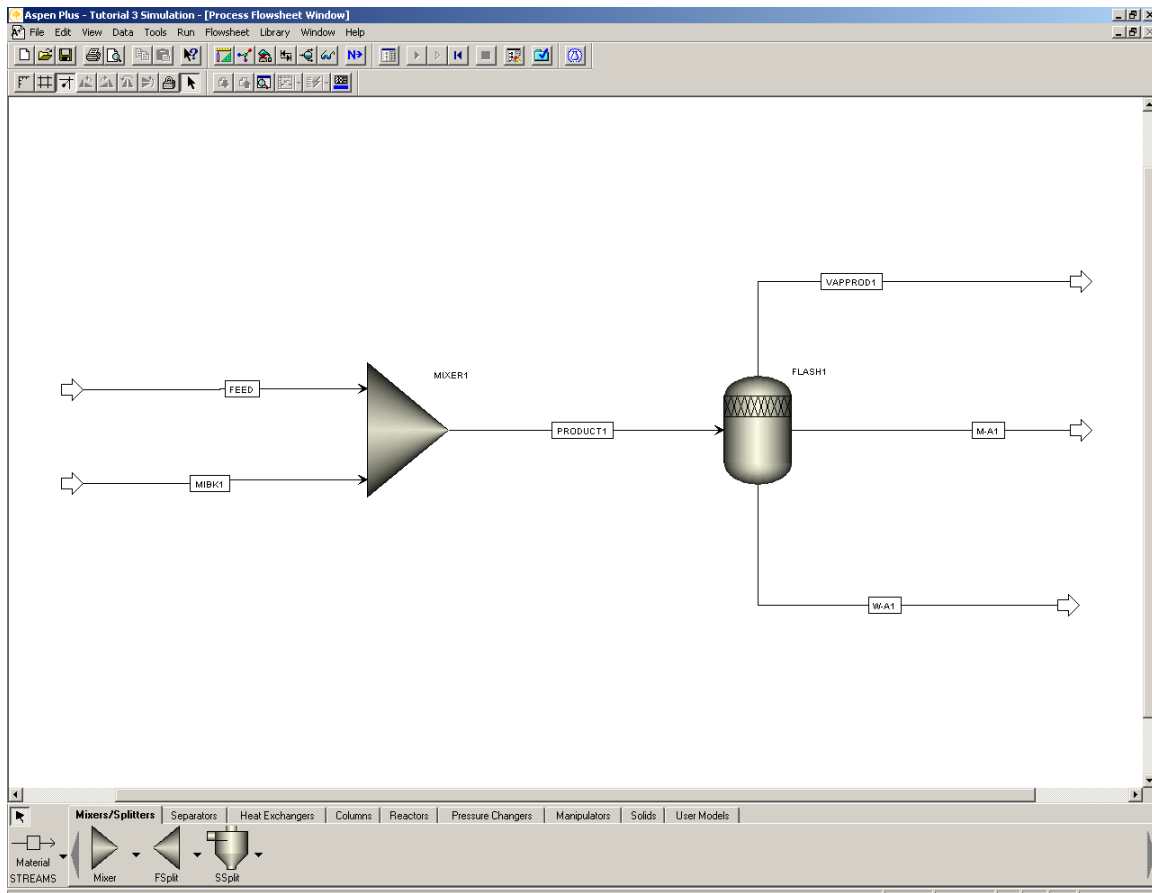
Figure 2: Completed Flowsheet

Updating the User Input:

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

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

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

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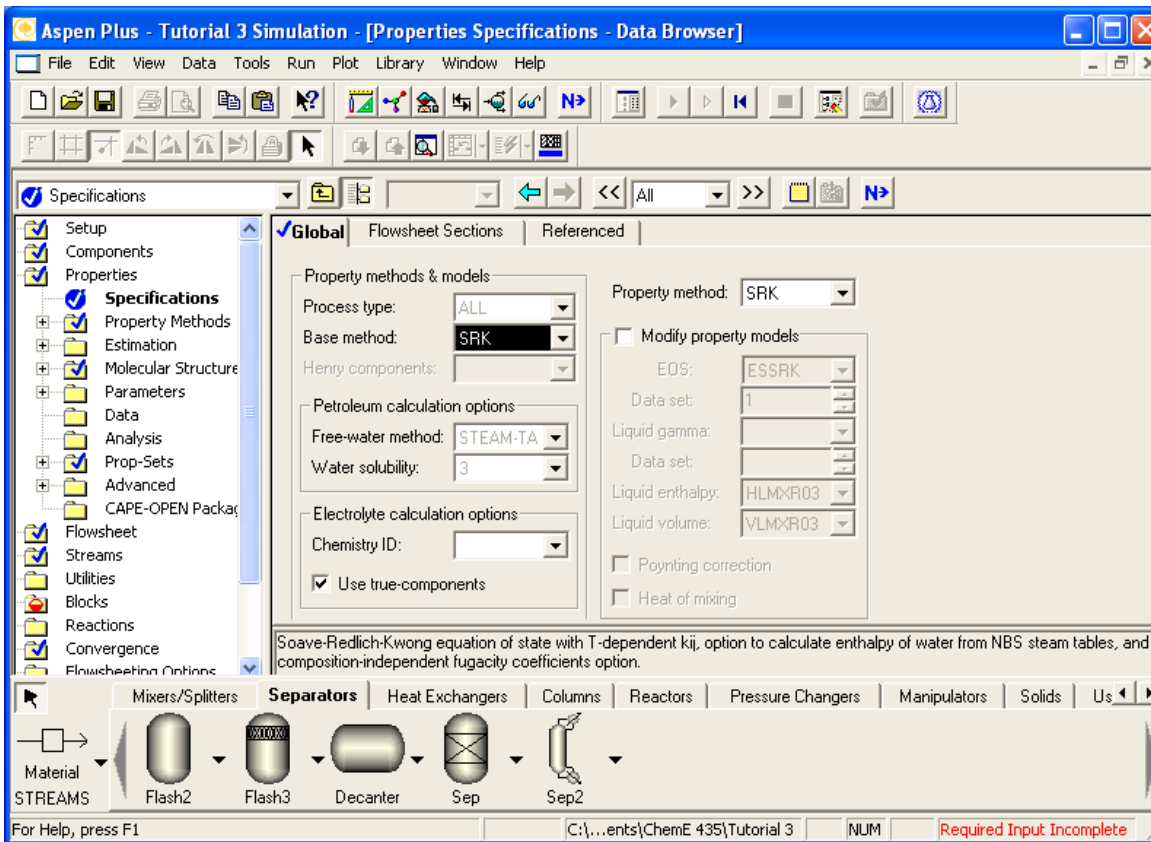

Figure 3: Thermodynamic Base Method

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

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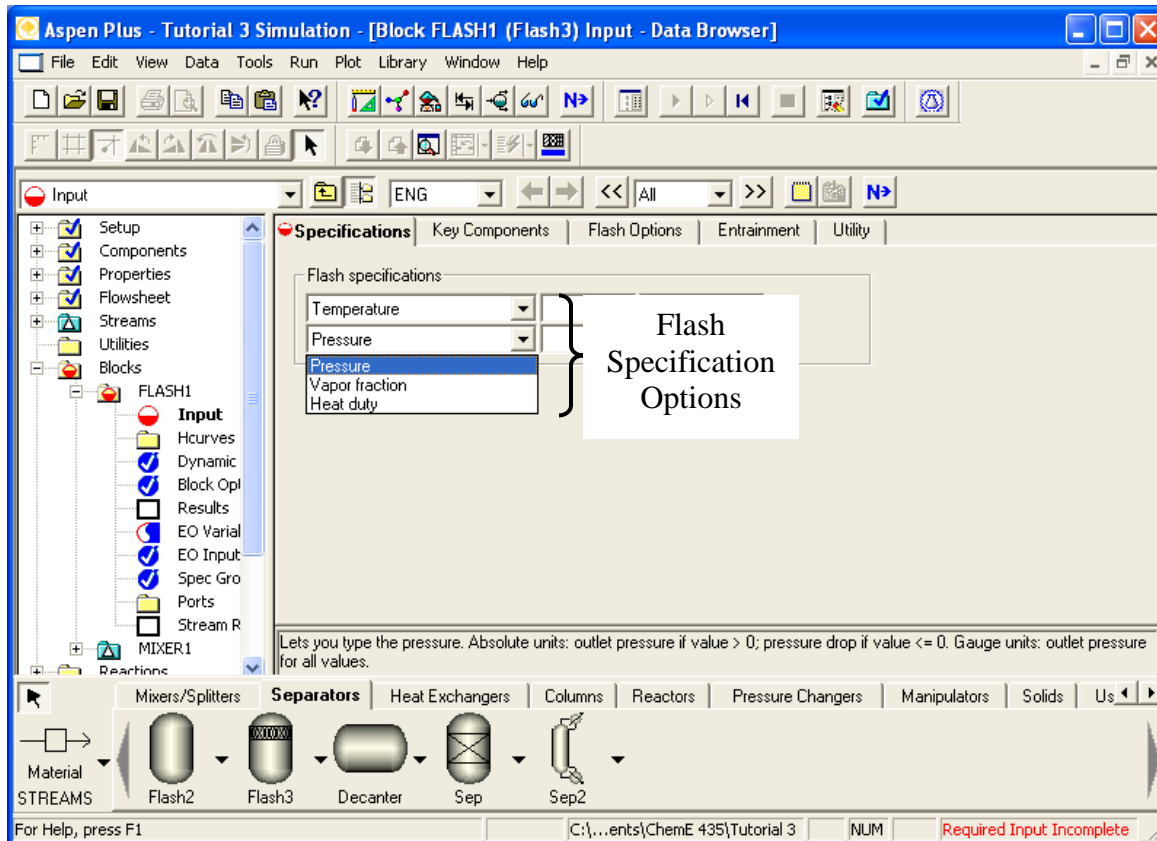
Figure 4: Flash Data Input Options

Running the Simulation and Checking the Results:

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

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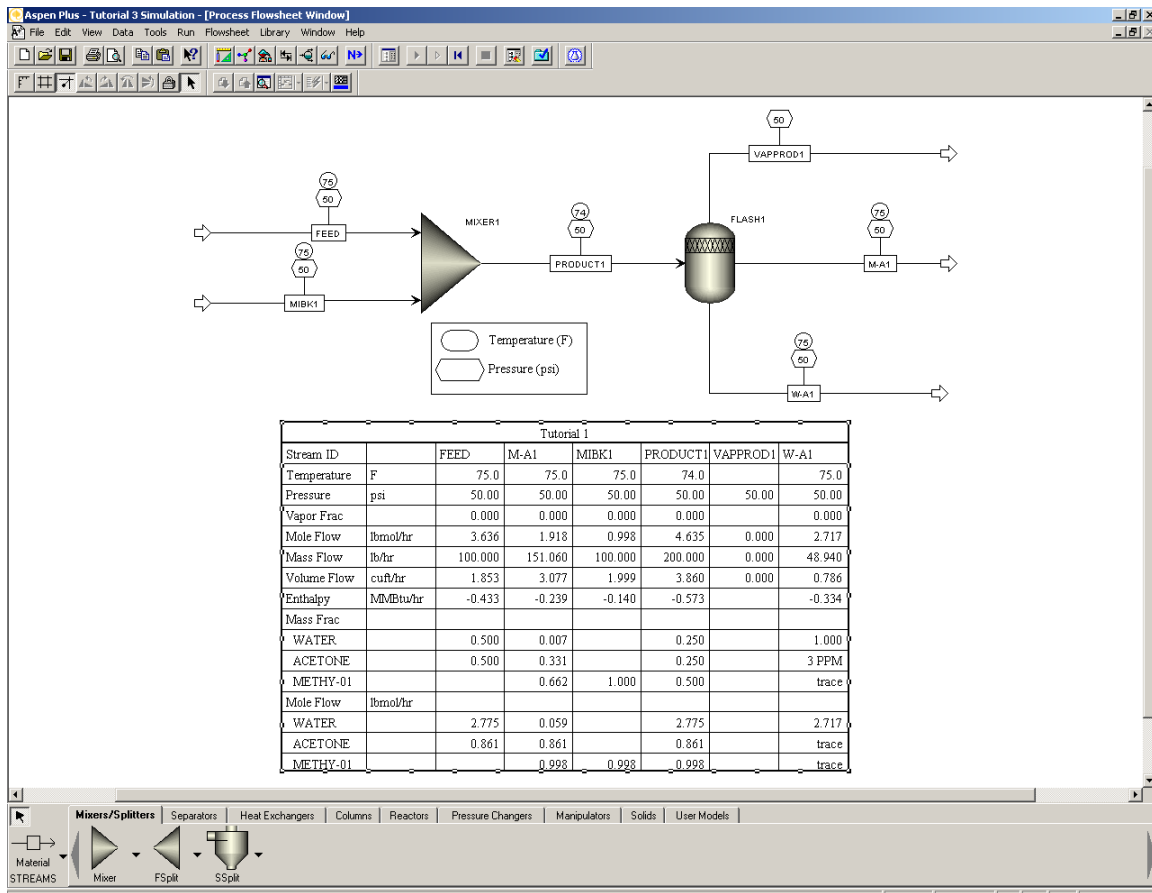
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Figure 5: Completed Process Flowsheet

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.
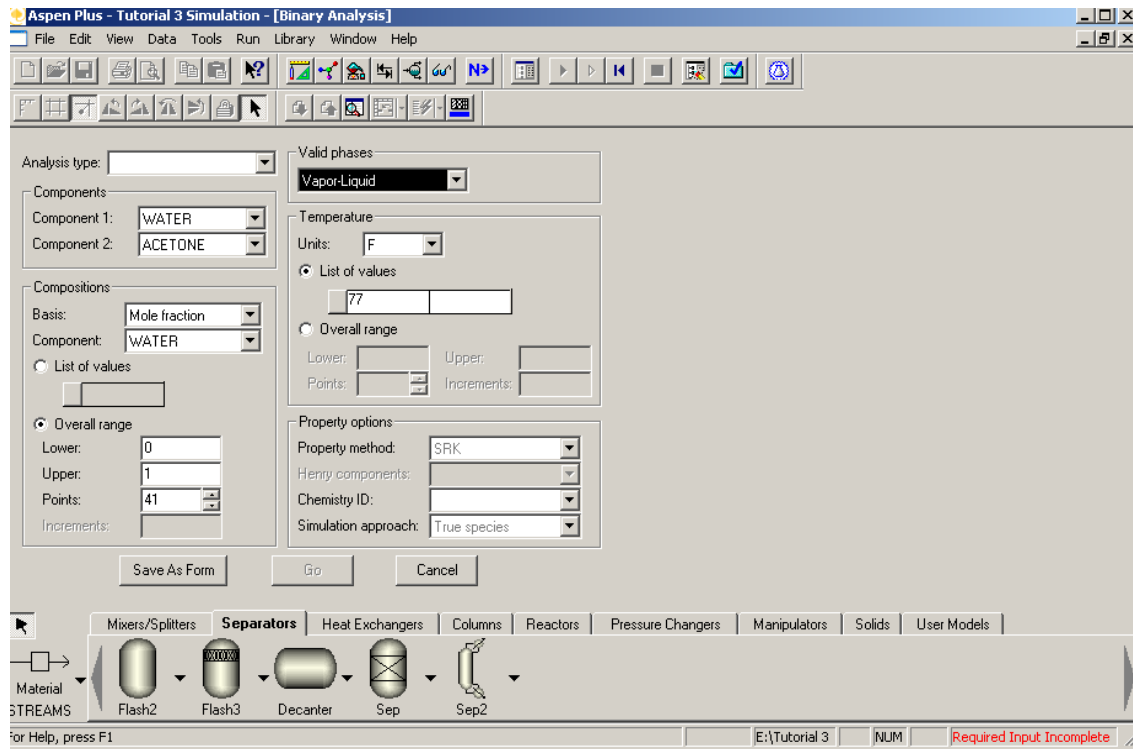
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Figure 6: Binary Analysis Window

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

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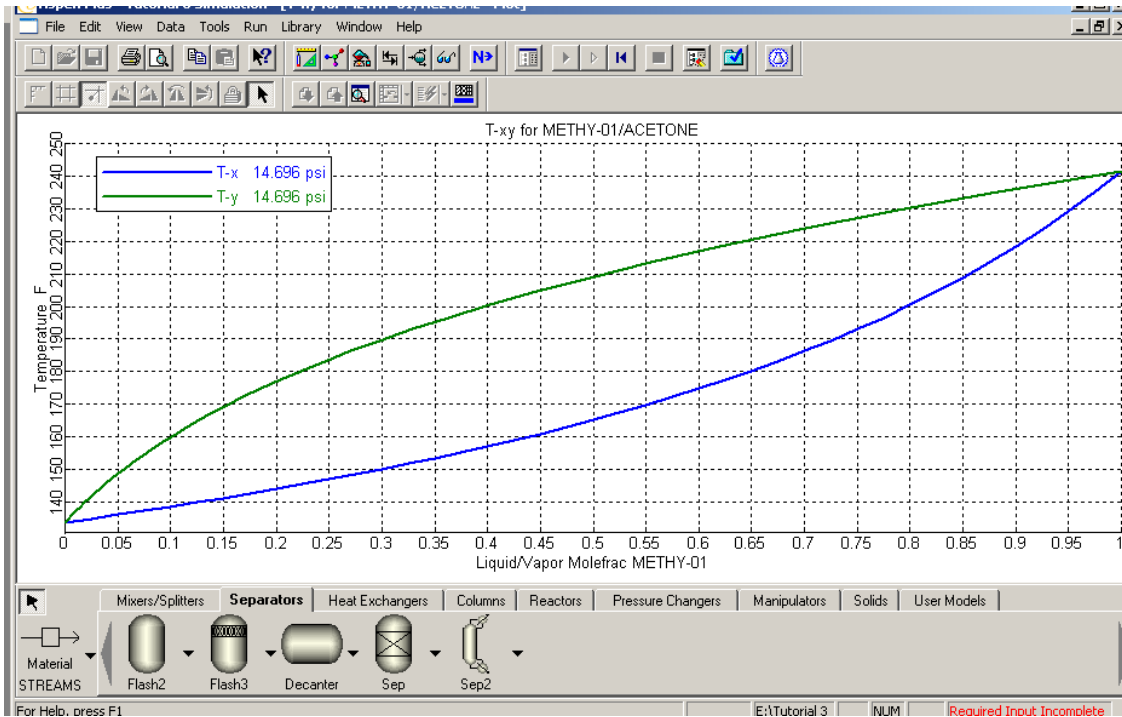
Figure 7: Txy Plot for MIBK and Acetone

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

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

In step 2 of the plot wizard you are presented with five options for variables that you can plot for this system. Gamma represents the liquid activity coefficient for the components and it is plotted against mole fraction. The remainder of the plot wizard allows you to select the component and modify some of the features of the plot that you are creating and upon hitting the finish button, your selected plot should open. Again, the plot can be further edited by right-clicking on the plot and selecting properties. In the homework for this week you will be turning in a plot of the liquid activity coefficient, so you can do that now if you would like. Otherwise, you can save your simulation for next week when we examine the various thermodynamic methods used by Aspen.
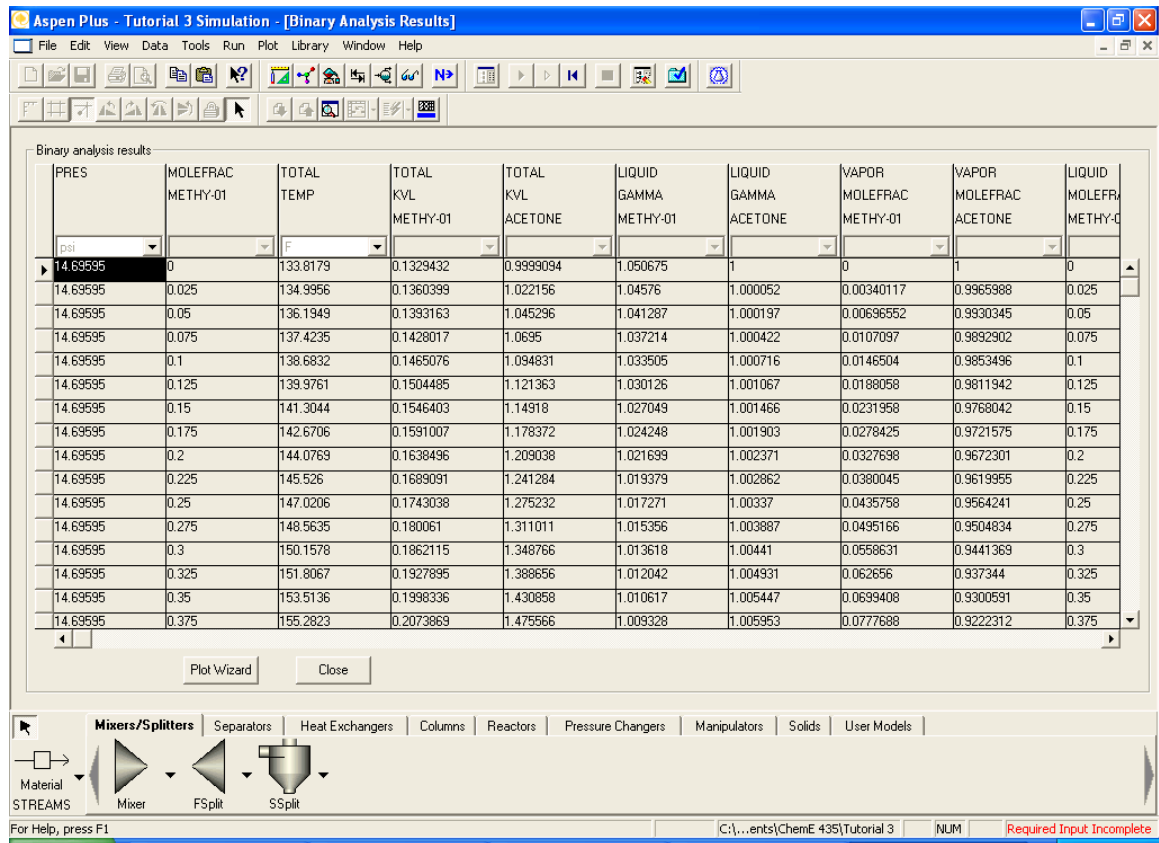
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Figure 8: Binary Analysis Results Window

Next week: Thermodynamic Methods

Tutorial #3 Homework

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).