Aspen Tutorial #3: Flash Separation

Outline:

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

Problem Description:

A mixture containing 50.0 wt% acetone and 50.0 wt% water is to be separated into two streams – one enriched in acetone and the other in water. The separation process consists of extraction of the acetone from the water into methyl isobutyl ketone (MIBK), which dissolves acetone but is nearly immiscible with water. The overall goal of this problem is to separate the feed stream into two streams which have greater than 90% purity of water and acetone respectively.

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

Adding a Flash Distillation Unit:

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

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

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

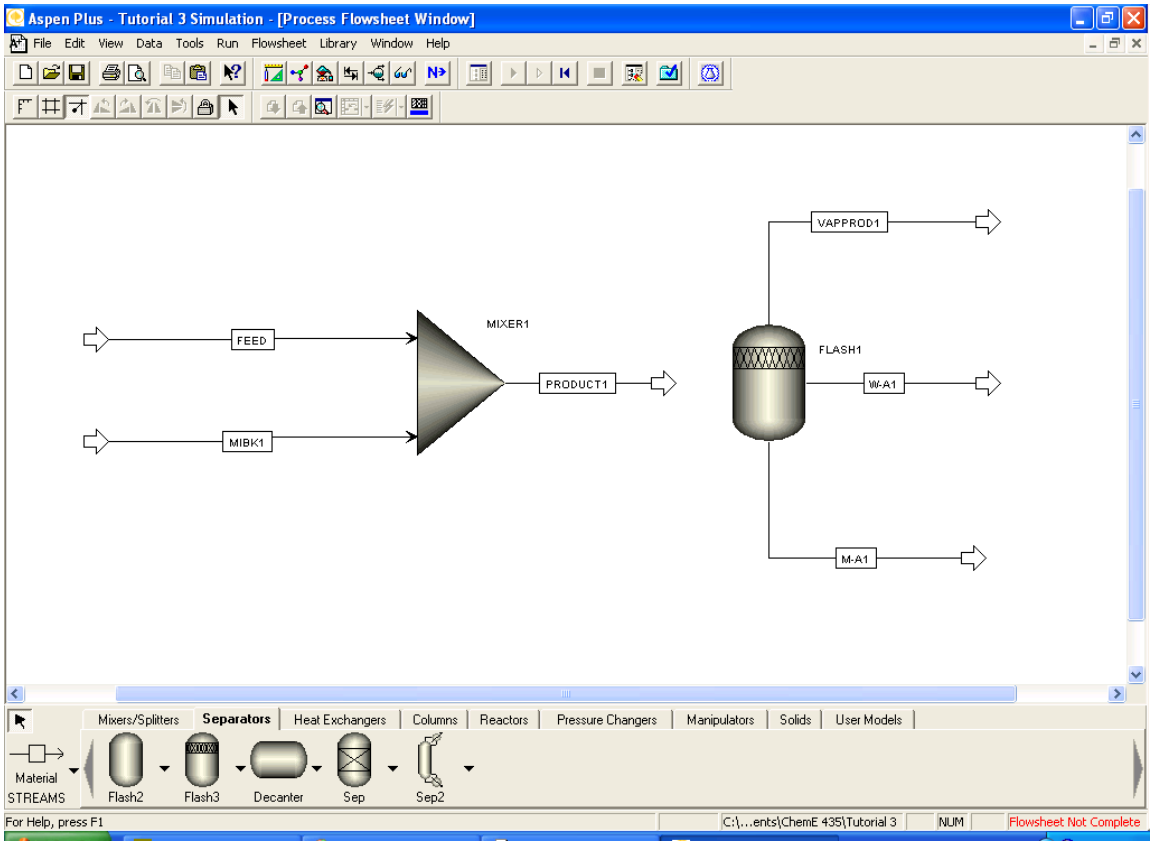


Figure 1: Flash Separator

To connect up the feed stream to your flash separator right click on the product stream from your mixer (mine is named PRODUCT1). Select the option Reconnect Destination

and attach this stream to the inlet arrow on the flash separator drum. After renaming your streams as you see fit, your process flowsheet should look similar to that in Figure 2.

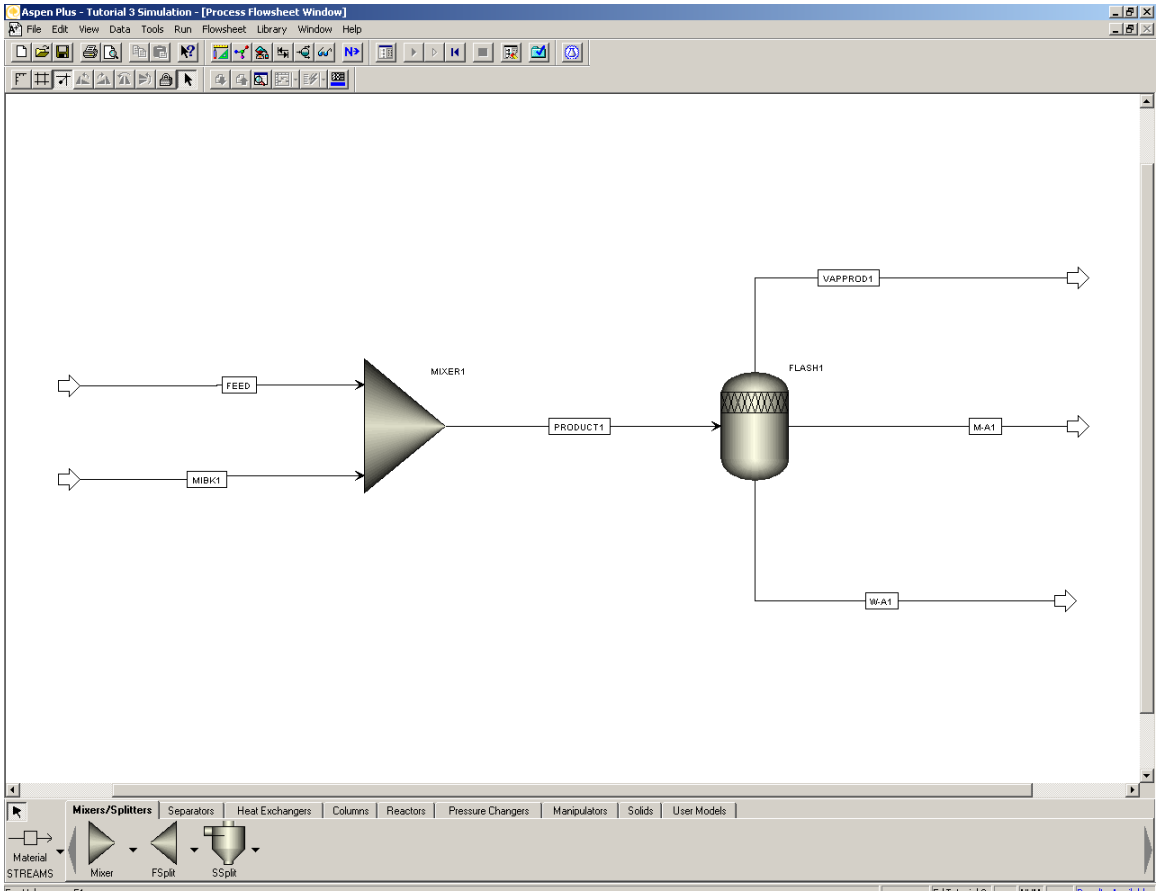


Figure 2: Completed Flowsheet

Updating the User Input:

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

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

In order for our simulation to properly model VLL equilibrium, we will need to change the thermodynamic method from IDEAL. In the data browser, select specifications under the Properties tab. Change the Base method from IDEAL to SRK (Soave-Redlich-Kwong equation of state) as shown in Figure 3. Next week we will be discussing the different thermodynamic methods, so this will not be discussed in depth now.

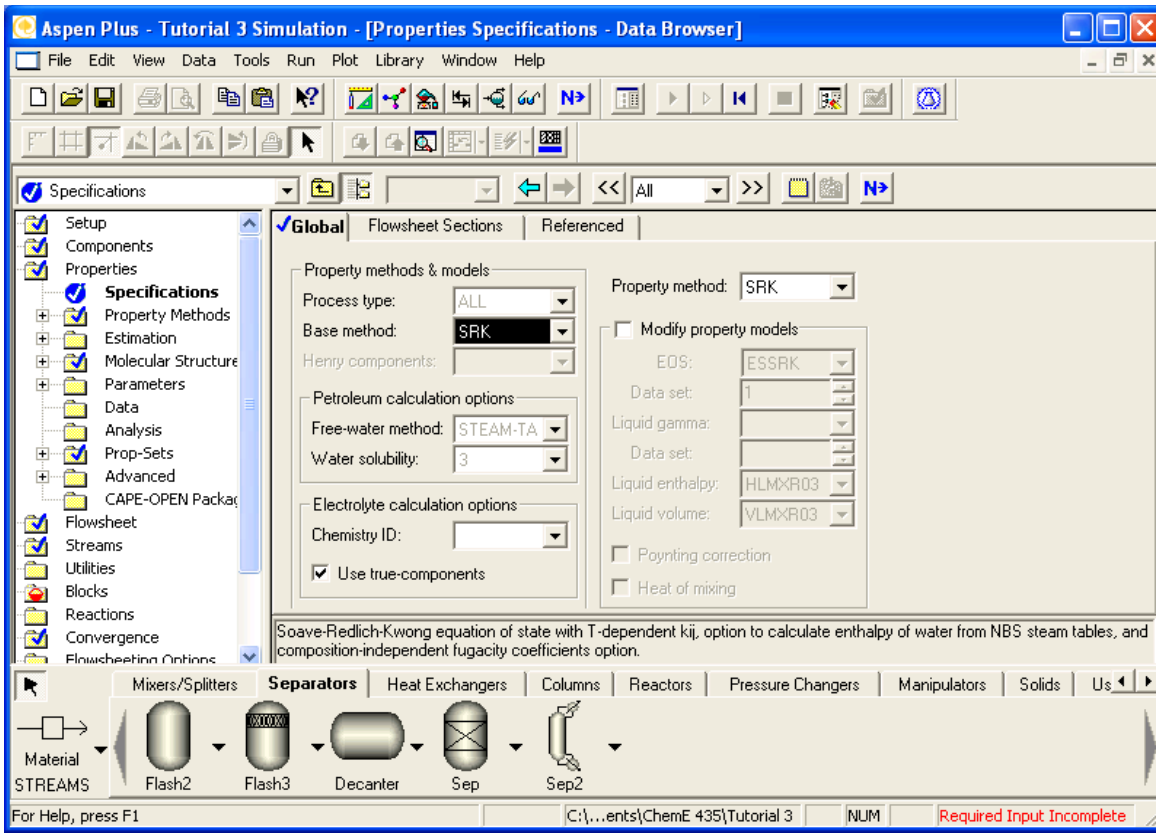


Figure 3: Thermodynamic Base Method

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

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

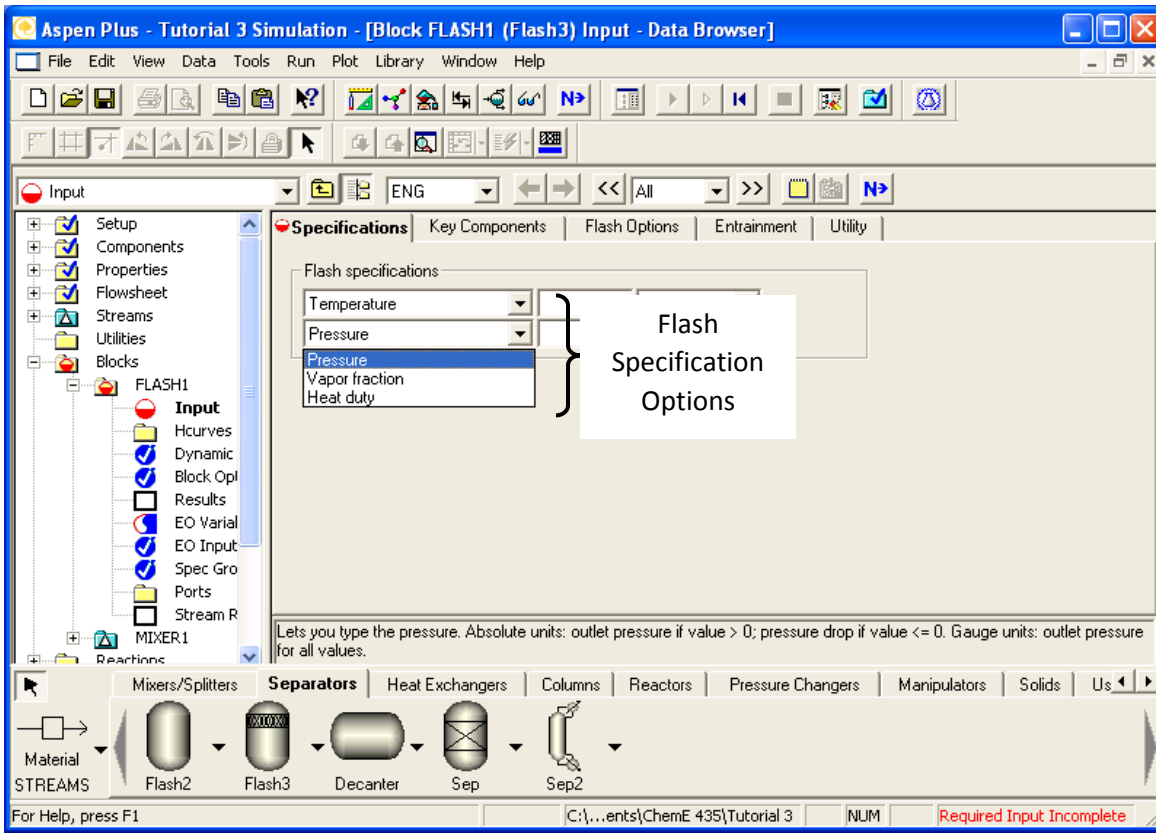
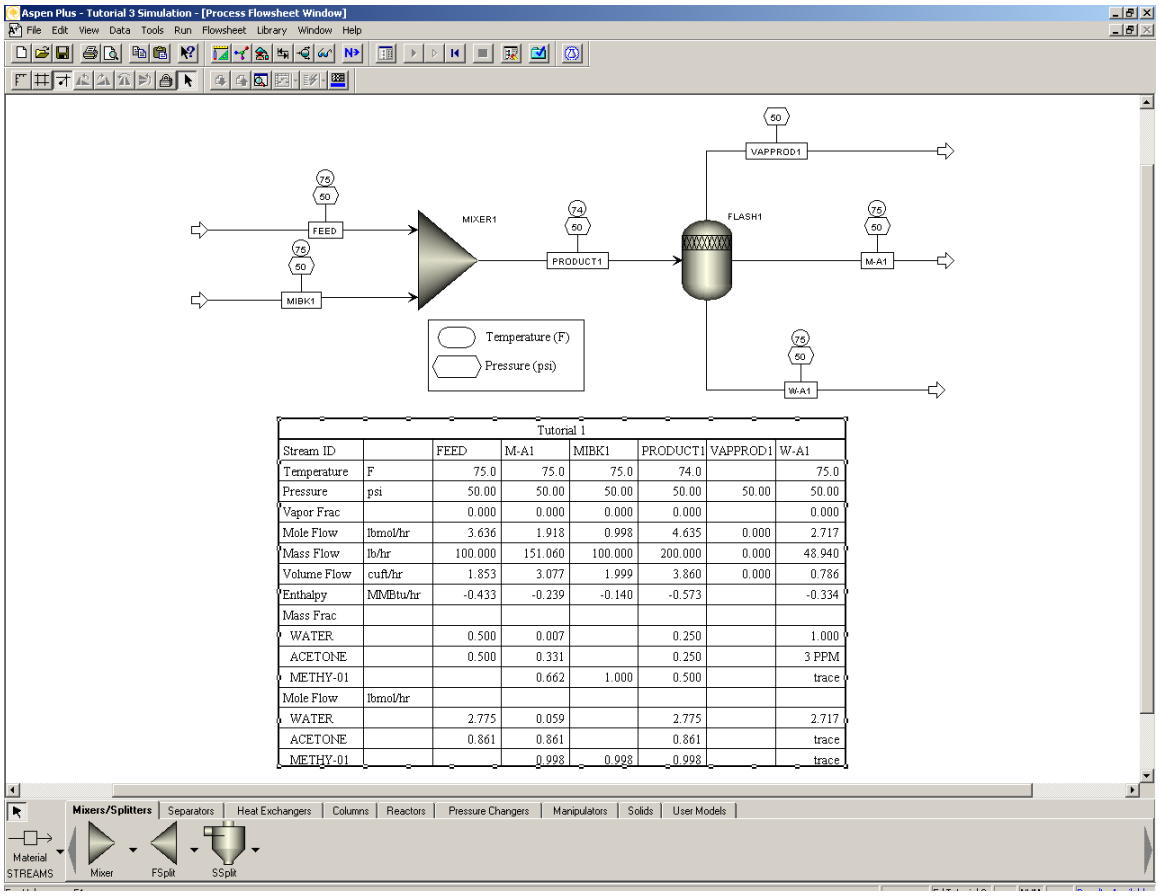


Figure 4: Flash Data Input Options

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).



Tutorial 1

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

Figure 5: Completed Process Flowsheet

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

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

Generating Txy and Pxy Diagrams:

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

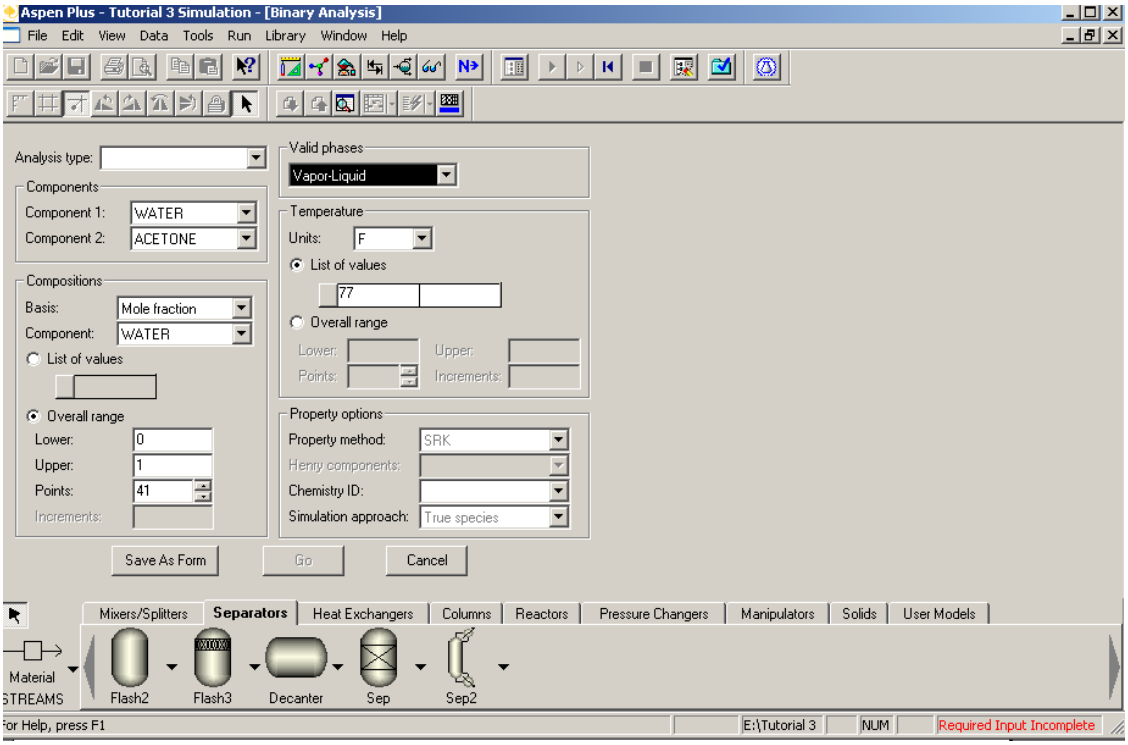


Figure 6: Binary Analysis Window

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

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

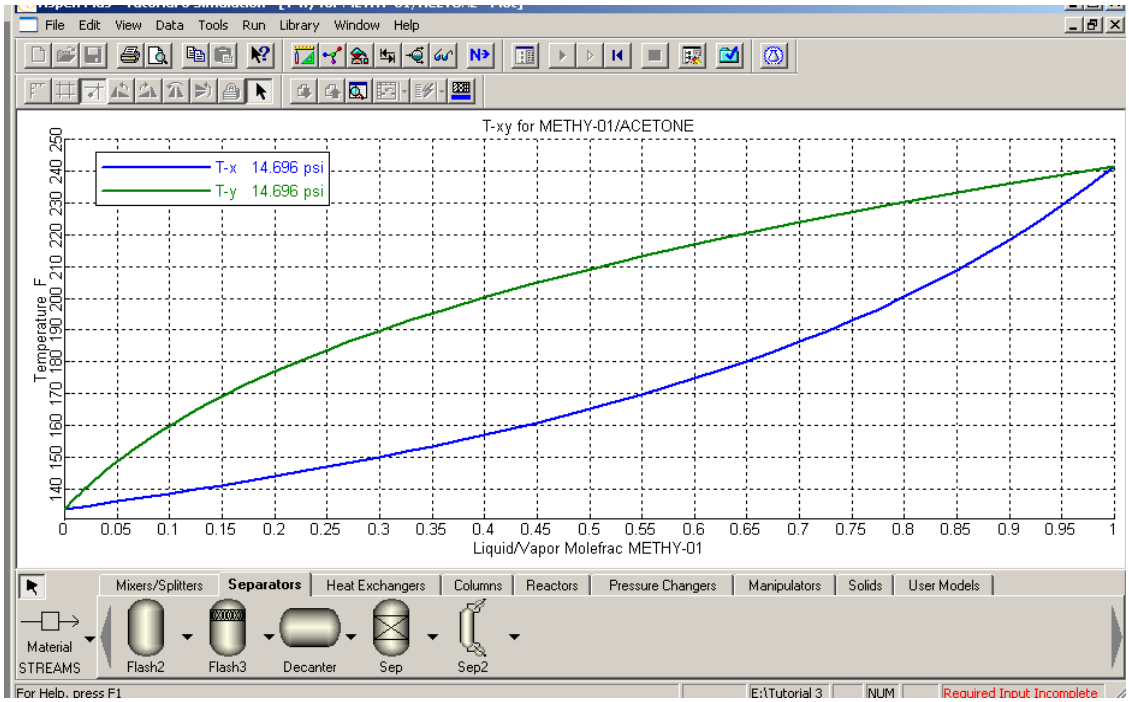


Figure 7: Txy Plot for MIBK and Acetone

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

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

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

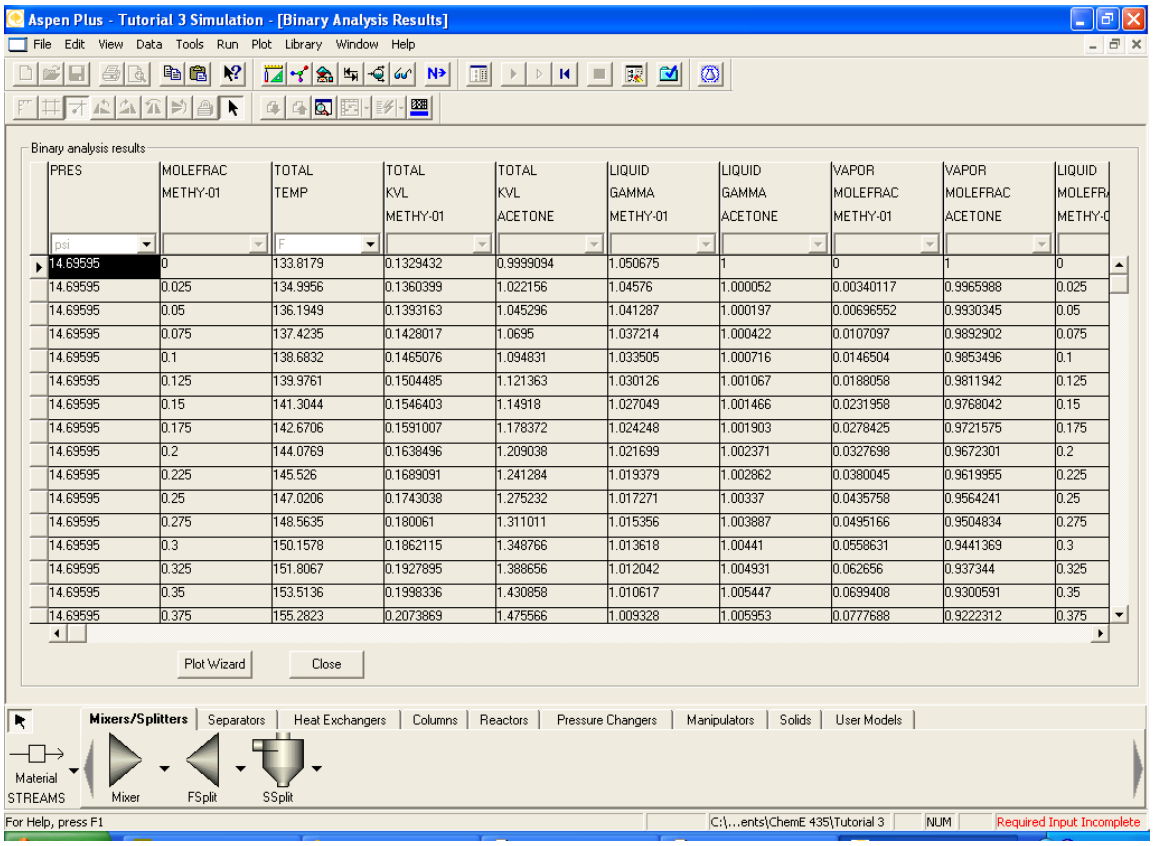


Figure 8: Binary Analysis Results Window

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).

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. Now, 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.

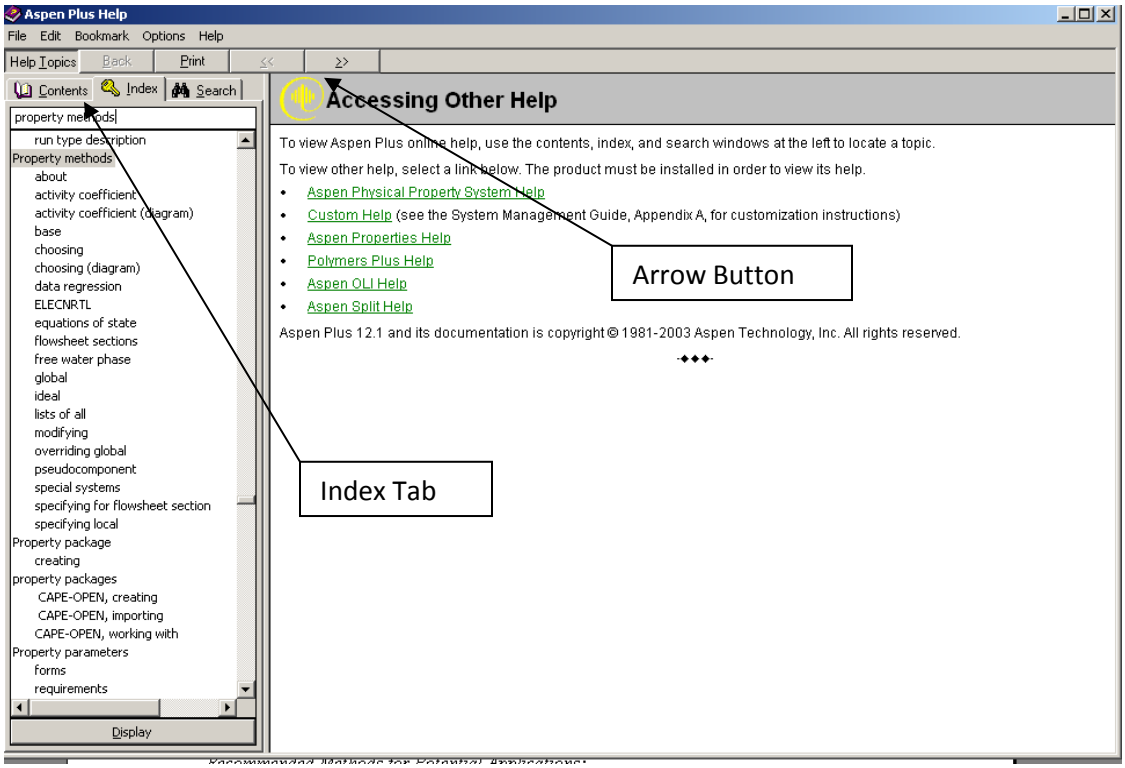


Figure 1: Aspen Plus Help

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.

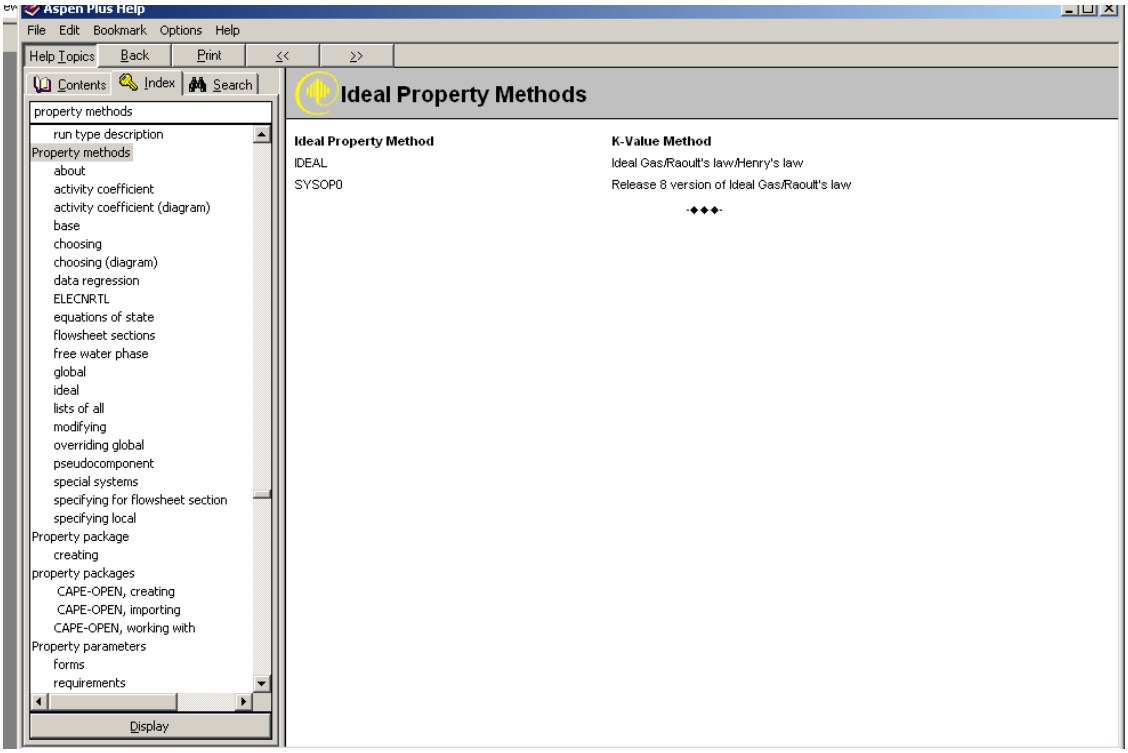


Figure 2: Ideal Property Methods

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.

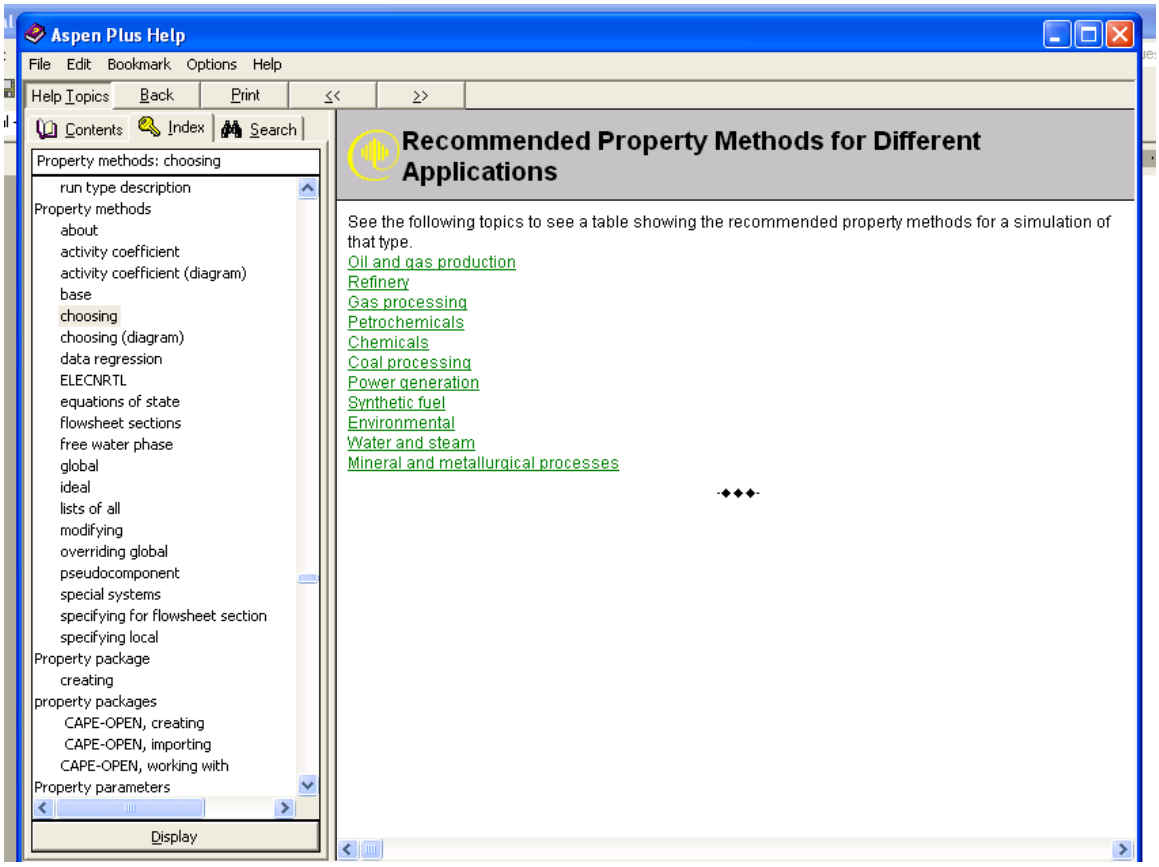


Figure 3: Recommended Property Methods for Different Applications

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.

Tutorial #4 Homework

Question:

Compare the simulation results from previous tutorial 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.

Exercise Problem

Question:

A 300 kmol/hr feed consisting of 20, 30, 10, and 40 mole% of propane, n-butane, n-pentane, and n-hexane, respectively, enters a flash chamber (Block: Flash2) at 15 psia and 50°F.

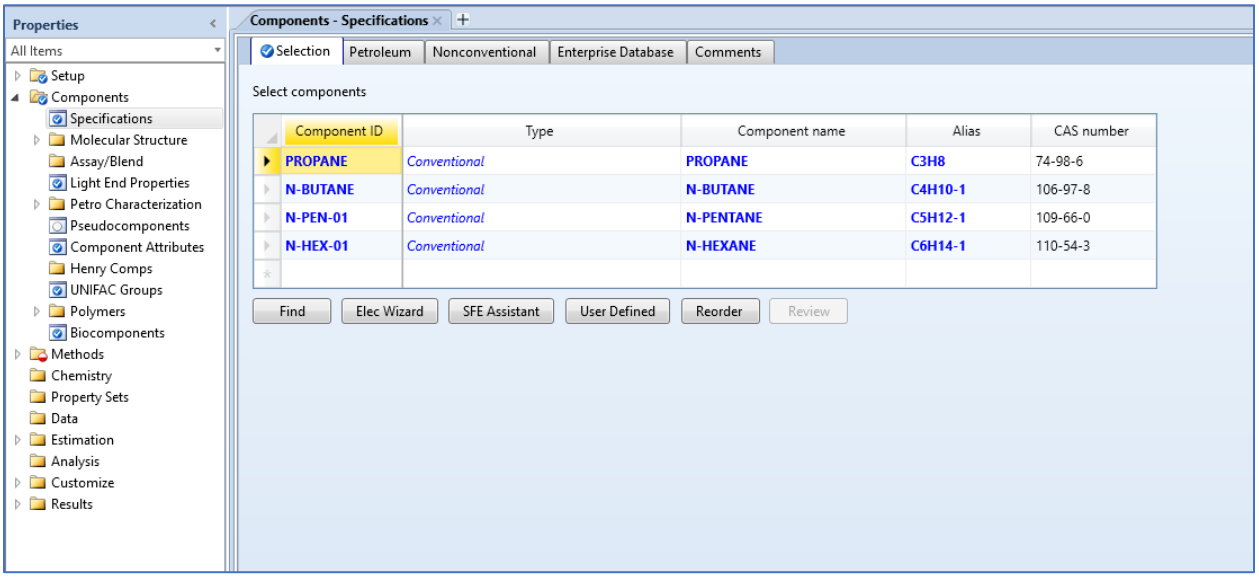
i. Compute the bubble point and dew point temperatures of the hydrocarbon mixture at 100 psia pressure.
ii. Consider that the flash drum operates at 100 psia and 250°F. Compute the composition of the exit streams.

Note: Use *SYSOP0 property* method for the study

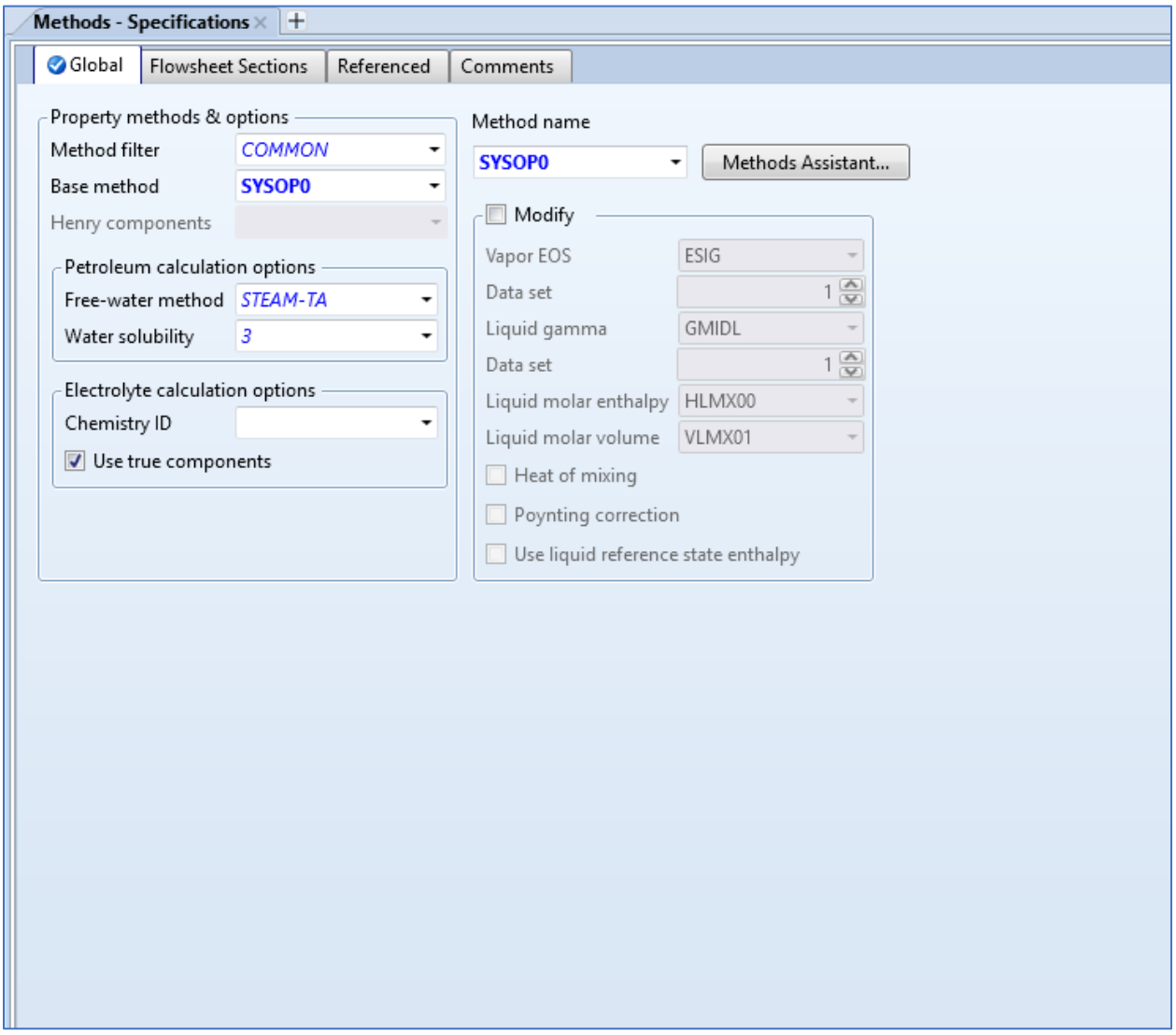
Solution:

For part (i)

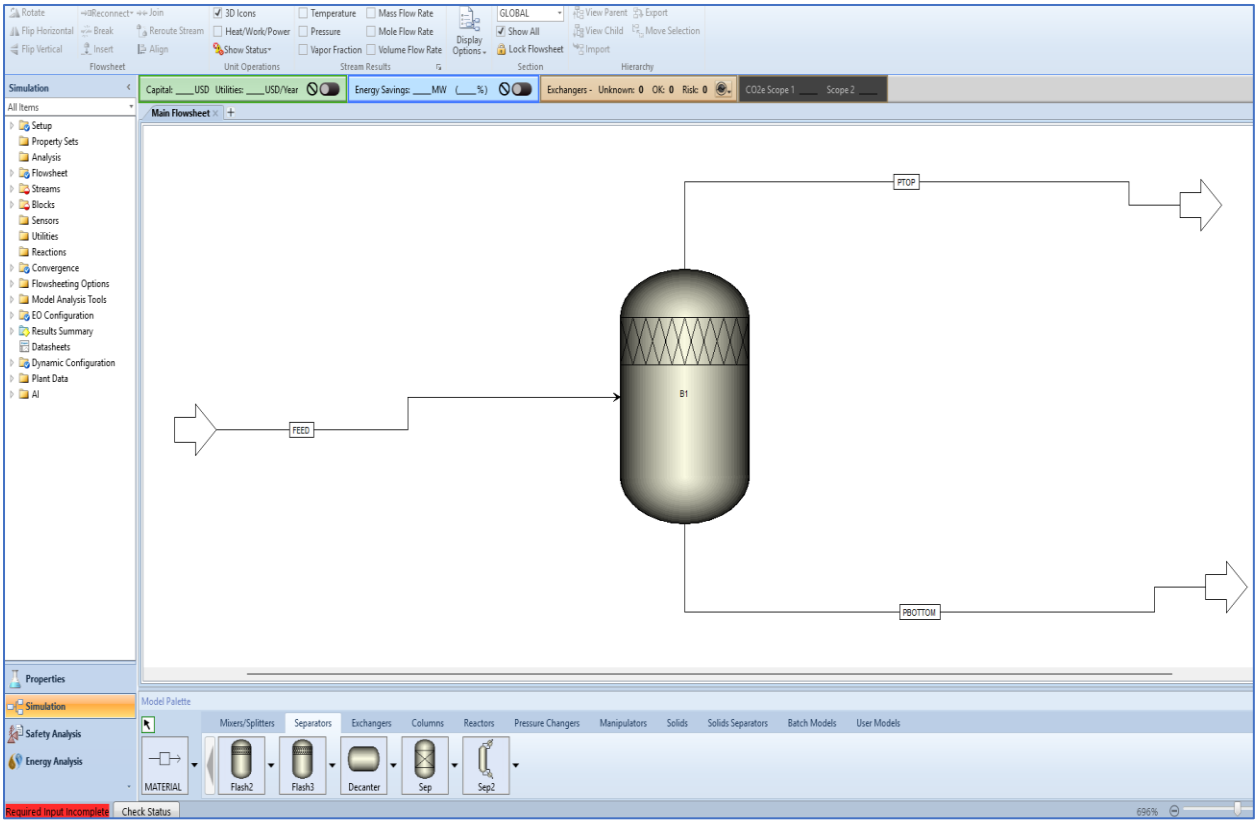
1. Open up a blank simulation and input the component specifications as mentioned in the question.



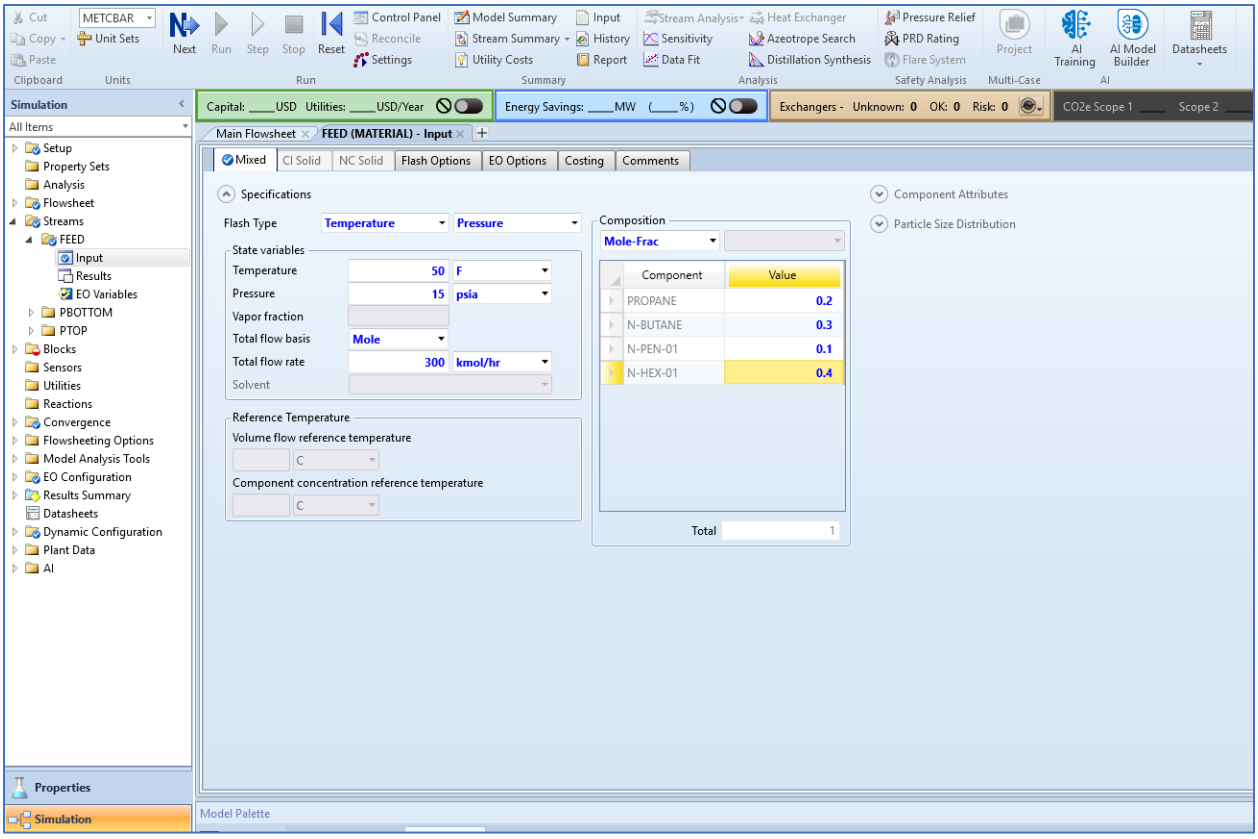
2. Click **NEXT** and choose the *Method Specification* as mentioned in the question. Click **NEXT** again and click on **Run Property Analysis/Setup** in the dialog box that appears. The Control Panel should open up without any error logs.



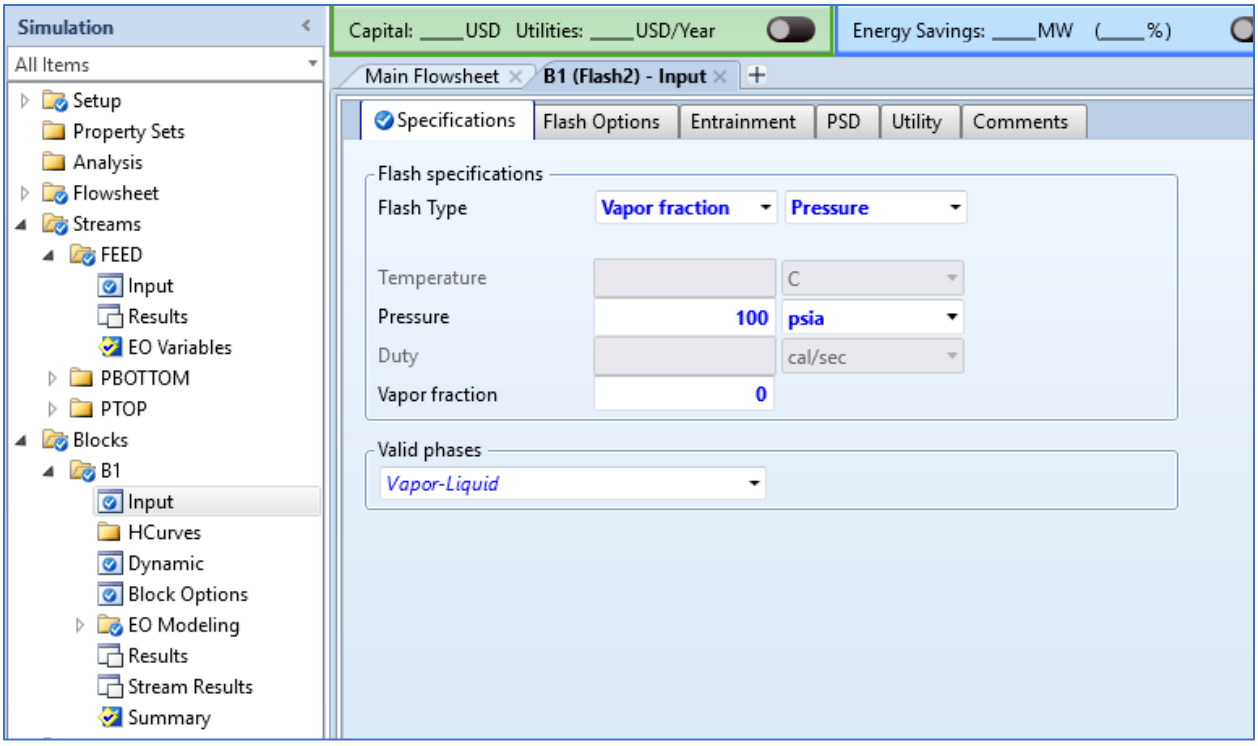
3. Now move to the *Simulation environment* of the *Navigation Pane* on the left side of your screen. You will land in the flowsheet window. Add a Flash 2 block and necessary material streams as shown below. Name the streams as: feed stream – FEED, top stream- PTOP, and bottom stream- PBOTTOM



4. Click **NEXT** and the input tab for the FEED stream will open up. Fill in the input as mentioned in the question.



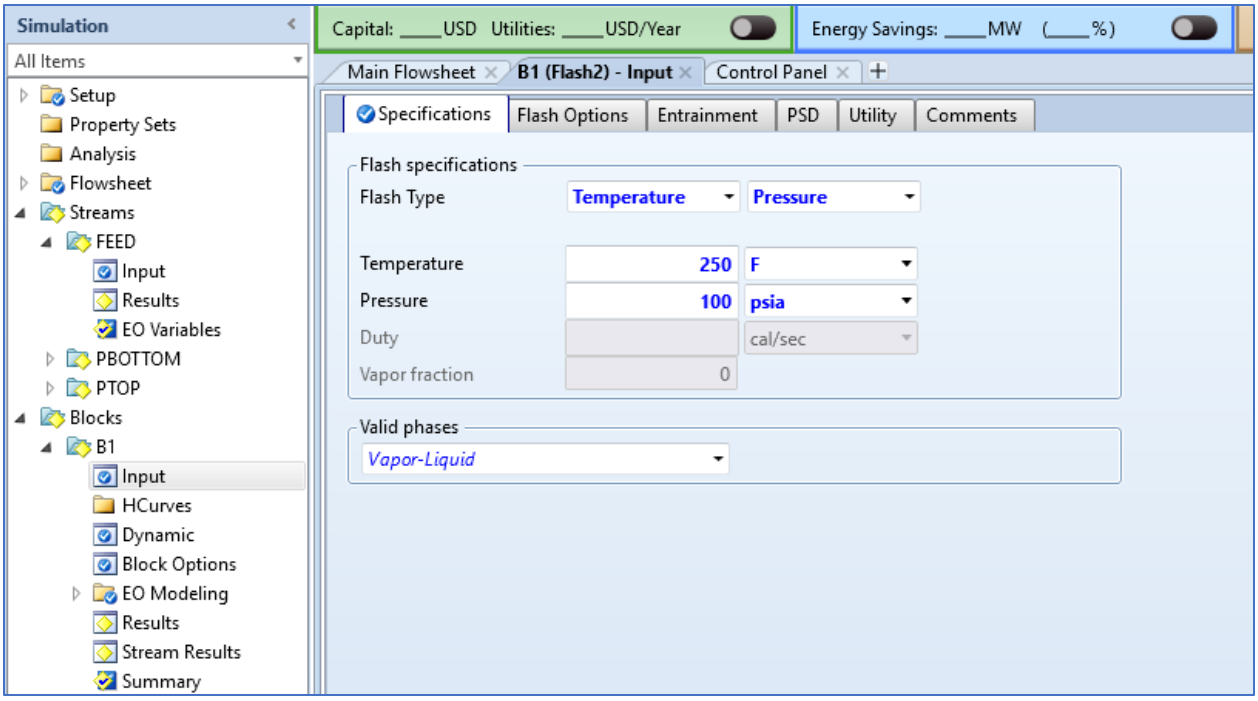
5. Click **NEXT** and you will be directed to the input tab for block B1 flash unit. For bubble point calculation, input Pressure as 100 psia and Vapor Fraction as 0. When bubble point is calculated whole of the mixture is in liquid state.



6. Click **NEXT** and run the simulation. The Control Panel should open up without any error logs. Now, in the *Simulation environment* on the Navigation Pane, select *Blocks/B1/Results.* The results for B1 block will open up. Note the outlet temperature. This shows the Bubble point temperature for the mixture.
7. Repeat the step 5 and 6 to calculate dew point temperature. Remember, for dew point temperature calculations, the vapor fraction is considered to be 1.

For part (ii)

1. In step 5 of previous part, input temperature and pressure values for flash specifications of B1 block as mentioned in question.



2. Click **NEXT** and run the simulation. The Control Panel should open up without any warning or error log.
3. Go to *Results Summary/Streams* on the Simulation environment of Navigation Pane to see the product stream output. You may add a stream table to the flowsheet by going to the *Stream Summary* Ribbon in the Quick Access Toolbar and clicking on *Send to Flowsheet* option.