Getting Started

Objectives:

1. Learn how to access Aspen Plus
2. Introduce the Aspen Plus interface
3. Learn how to draw a process flowsheet and input data
4. Learn how to run a simulation and view results

Accessing Aspen Plus

There are two ways to access Aspen Plus. The first method is to directly select it from the Start Menu by going to AspenTech>Process Modeling V7.2>Aspen Plus>Aspen Plus User Interface. Choosing this option will directly open Aspen Plus for use.

The second method is through the Process Engineering Console. The Process Engineering Console is an interface provided by AspenTech that combines several useful applications in one place. A snapshot of the Process Engineering Console is shown in Figure 1.

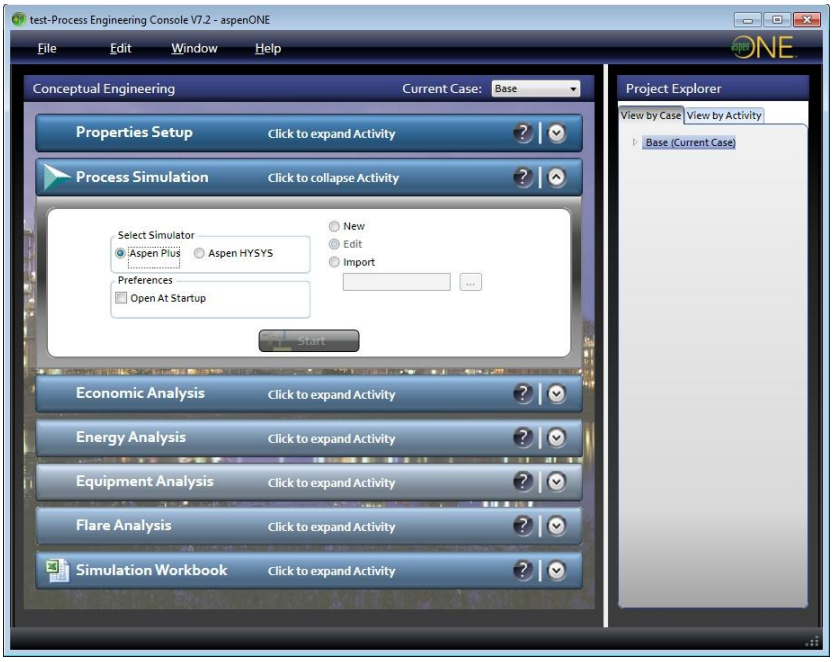


Figure 1. The Process Engineering Console.

As you can see, the Process Engineering Console works with what it call a *project*. A project can undergo several *analyses* as shown in Figure 1 from properties estimation, the simulation itself, to economic and energy analysis and others.

To start Aspen Plus from the console, collapse the Process Simulation tab, select Aspen Plus option, select New option, and click 

.

Aspen Plus Interface

Once you start a new simulation in Aspen Plus, the window shown in Figure 2 appears. As you can see, the window has the typical components of Microsoft Windows interface. In addition to the typical components of the interface (Open, Save…), the window has many menus and toolbars that will assist you in building, running, and debugging the simulation. Some of the main components are indicated on the Snapshot in Figure 2.

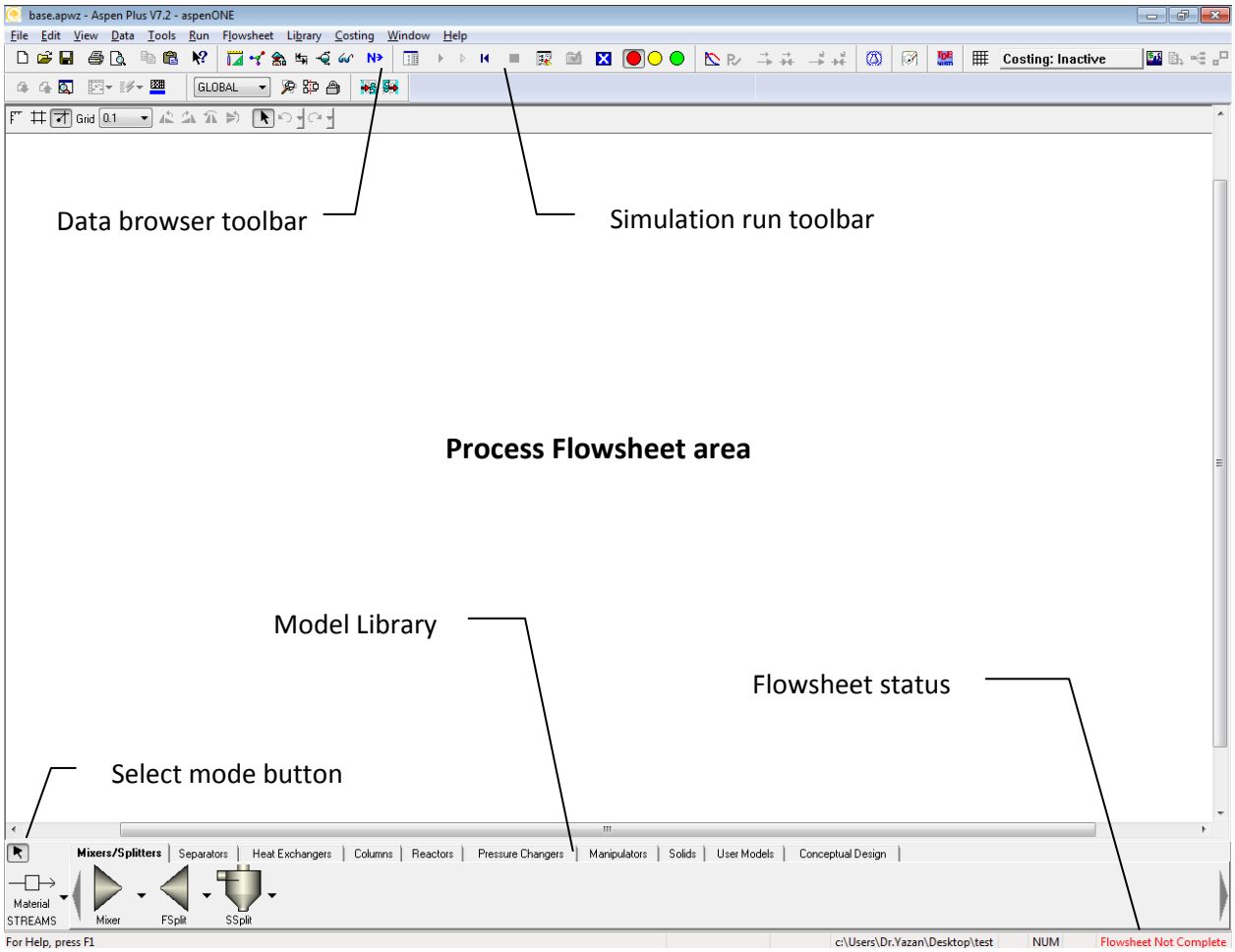
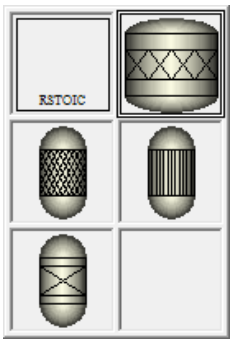


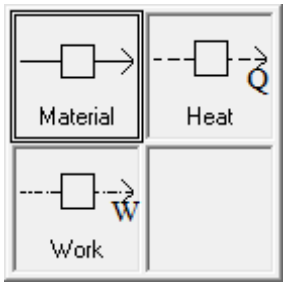
Figure 2. Aspen Plus User Interface.

In terms of building your simulation, the most important parts are:

1. Model Library: This is basically where the unit operations (plus other models) are presented. As you can see, the Model Library is divided into tabs, according to the type of unit operation involved. Under each tab, there are several models (icons) each of which represents a certain type of that unit operation. For example, under the Reaction tab you will see the RStoic, RYield, REquil, RGibbs… models, each of which represents a different model to calculate the reaction products. Notice also that under each model, there are several icons that you can use. For example, the RStoic model has the icons shown to the right. These icons are only for representation purposes, they all do the same function. In fact, once an icon is placed, you can easily switch between them by clicking Ctrl+K.



2. Select Mode button: Once you place a model (or models) on the flowsheet, you can adjust the model's icon position, resize it, or delete it, or you can draw process stream connections. If you want to do any adjustments to the icon, you need to make sure the Select Mode button is clicked. If, on the other hand, you want to connect process streams to the model, you need to click the STREAMS button (located below the Select Mode button).
   By default, clicking the STREAMS button will activate the Material stream, which is similar to a process stream in process flowsheet. Material streams contain all the information about what is being transferred in that stream in terms of composition, flow rate, and other thermodynamic and physical properties. Other types of streams in Aspen Plus (and simulation software in general) are the energy and work stream. You will notice that next to the STREAMS button there is a small downward triangle. If you click on this triangle you will see the three types of streams available for you: Material, Heat, and Work. The Heat stream is used when heating/cooling is taking place or when we want to transfer heat from unit to another. Work streams are used when work is supplied or extracted from a unit (*e.g.*, compressor or turbine) or if we want to transfer work from one unit to another.



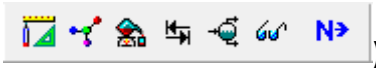
3. Data browser toolbar (): the icons on this toolbar will open different pages of a window called Data Browser. The Data browser is where all the process information is input from the thermodynamic model used, the components, physical properties, streams information, units' information, and other.
   The data browser is divided into folders, under each folder there are several sheets, and in each page there are several tabs. Within these tabs you can control all features of your simulation. You will learn how to use different parts of the browser as we go on. The Data Browser is shown in

Figure 3.

4. Simulation Run toolbar (): This toolbar contains buttons that will allow you to run, pause, stop, and debug your simulation once you have completed the flowsheet creation. The toolbar will have different buttons activated/deactivated depending on the status of the flowsheet.

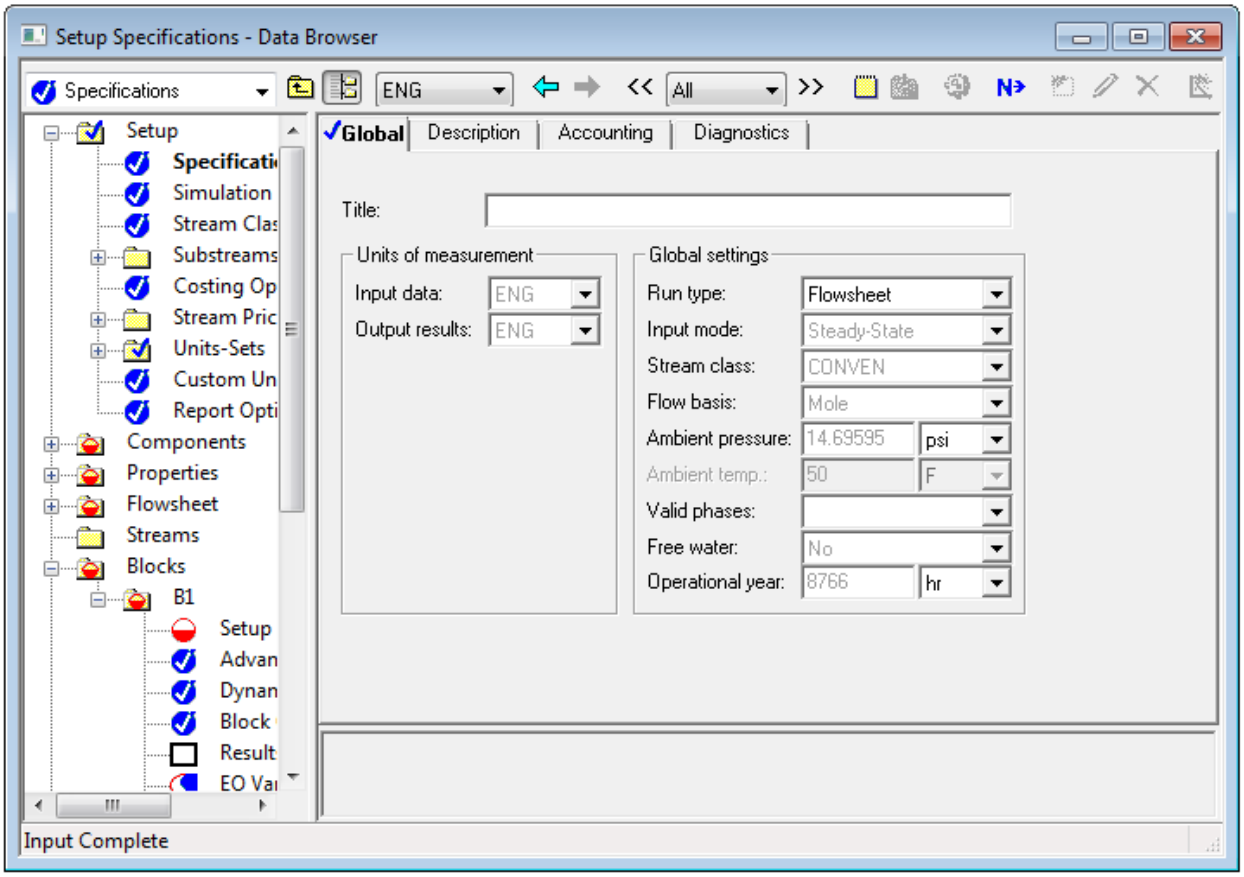


Figure 3. Data Browser.

5. Flowsheet Status bar: This is located at the lower right corner of the window and indicates the status of the flowsheet. When you start a flowsheet, the message shown will be "Flowsheet Not Complete", indicating that there are missing streams that need to be connected. Once you make all necessary connections, the message will change to "Required Input Not Complete", indicating that you have not specified all required inputs. There are several messages that will appear as you work with your simulation, but, in general, your ultimate goal is to get the "Results Present" message, indicating that the simulation was performed successfully.

As you use Aspen Plus more, you will get to learn more features and aspects of the interface. For now, the above five components are enough to create our first simulation.

Remember always to use the help provided with Aspen Plus when you are in doubt or when you are not sure how to perform certain tasks. The help can be accessed from the Help menu or via the Help button ( ).

Drawing a Flowsheet

We will start by drawing a simple flowsheet. The flowsheet we will draw is for a simple extraction process in which acetone is removed from water using methyl isobutyl ketone (MIBK). In this process, a stream containing water/acetone mixture is mixed with a stream of MIBK. The resulting mixture is then sent to a decanter (3-phase separator) where the organic phase (MIBK-acetone) is separated from the aqueous phase (water-acetone). The process flowsheet is shown in Figure 4. As you can see on the flowsheet, enough information has been provided to completely specify each input stream. This includes the flow rates, composition, temperature and pressure. Other options for specifications exist, for example, flow rates of each constituent, temperature, and vapor fraction. As long as we have enough information, any combination of information is acceptable as long is the stream is fully defined.

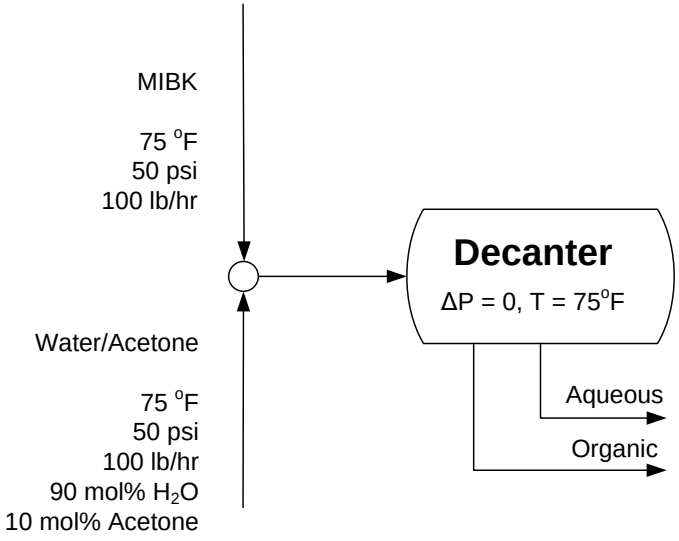
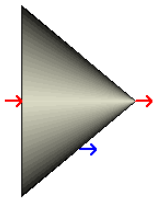


Figure 4. Acetone extraction from water using MIBK.

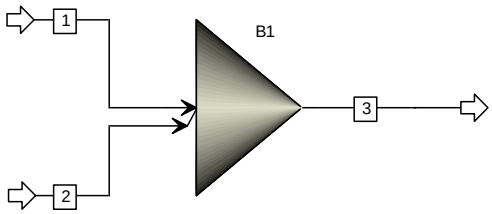
Recall when you studied material and energy balances that you can only solve a flowsheet if it has a zero degrees of freedom. Aspen Plus provides instantaneous feedback on the degrees of freedom as you build your simulation through the status bar messages. A process if fully specified when the message “Required Input Complete” is displayed in the status bar.

To draw the above flowsheet do the following steps:

1. Start by placing a mixer unit in the flowsheet. The mixer is available from the Model Library “Mixers/Splitters” tab. Select the Mixer Model (all icons will work) and place it on the flowsheet. This is the only unit needed in this simulation.

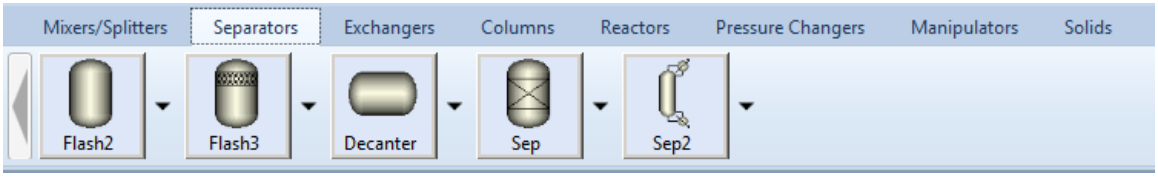


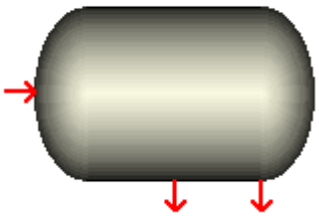
2. Connect two inlet and one outlet streams. To connect streams select the Materials STREAMS button and start drawing. An input stream is drawn by clicking on an empty area of the flowsheet and connected to the unit. In order to connect a stream to the model, you need to make sure an inlet is available. Notice that we select the Materials STREAMS button and put the cursor close to the unit, Aspen Plus will show you all available inlets and outlets (as shown in the figure to the right). The arrows in red represents one (or more) required input and output streams, while the ones in blue represent optional inputs and outputs. In this exercise we want to draw to input streams (notice that both will go to the same inlet port) and one output stream, as shown below.



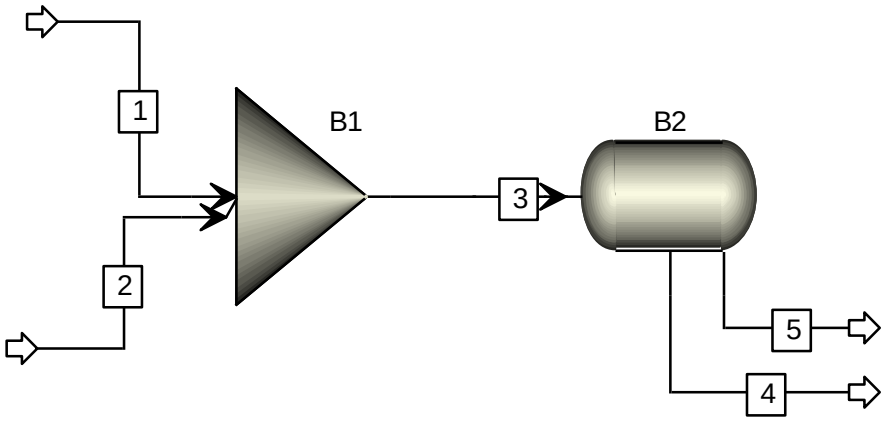
Notice that Aspen Plus has automatically named and numbered the streams and blocks. If you like to change the name of any stream or unit, right-click the stream (or block) and select Rename Stream (or Rename Block) or click Ctrl+M. This will open a popup window in which you can change the name. Also notice that you can change the way streams are drawn by selecting it and dragging the ends or elbows to where you want them to be.

3. Next, we need to draw the decanter. Like flash tanks, decanter is a phase-based separator. Simple phase-based separators are available under the “Separators” Library.





These include simple flash tanks (called Flash2 which is a vapor-liquid separator), 3-phase flash tanks (called Flash3, which is a vapor-liquid-liquid separator), decanters (called Decanter which is a liquid-liquid separator), and special separators (Sep and Sep2). You can read more about each separator by going to the Help>What's This? menu then clicking on the block you would like to learn about. In our case, we will use the decanter (shown to the right). This block is used to separate two liquid phases without a vapor phase, which corresponds to the system we have at hand. To add a decanter, click on the Decanter block and place it on the flowsheet, then make the required connections as shown below. In order to connect stream 3 to the decanter, right click on the stream and select Reconnect Source (or you can double click on the white arrow,  , at the end of the stream) then connect it to the input of the decanter.



Now we have finished drawing the simulation flowsheet. You can notice that the Status Bar message has changed from “Flowsheet Not Complete” to “Required Input Incomplete”. In the next part we will learn how to input the required data.

Inputting Required Information

The next step in building the flowsheet is to input the required information, which can be done through the Data Browser. To open the Data Browser, click on the Data Browser Icon () located on the Data Browser toolbar. This will open the Data Browser window in which you can input the required information.

There are three basic information that must be provided before we can run the simulation:

1. The thermodynamic model that will be used to estimate the components properties.
2. The input streams specifications.
3. The blocks specifications.

When you click the Data Browser button, the window in Figure 5 appears. Notice the folders tree to the left has different icons representing the status of that folder. You can check the Help topic "Status Indicator" for a complete list and definition of each icon. In general, before we can run the simulation we need to provide an input to all forms with a red circle icon (and). Any folder or form with a half-filled red circle indicates missing input. These icons will change to have a blue check (and) when the input is complete.

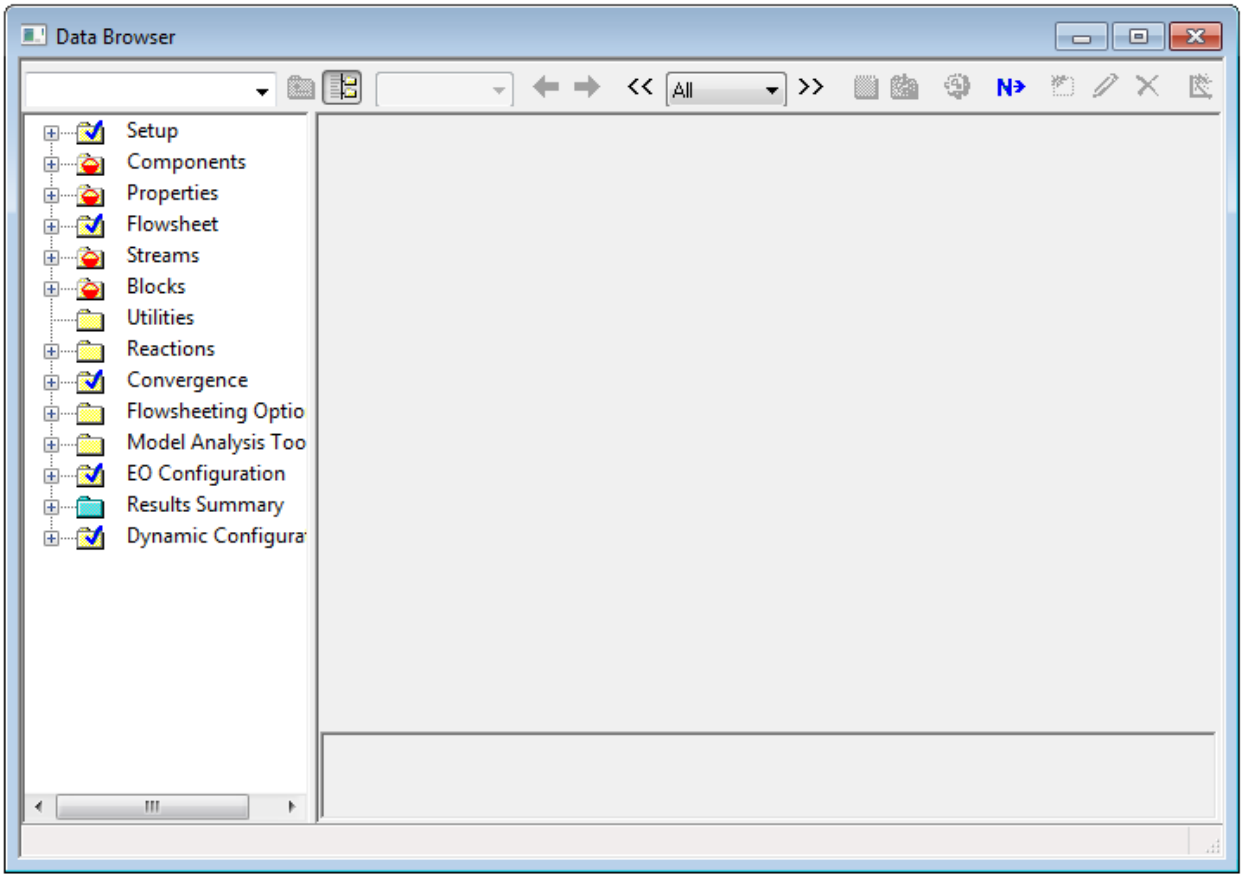


Figure 5. Data Browser.

In our simulation we see that the Components, Properties, Streams, and Blocks all have missing information. This means that we need to define the components we want to use, define the thermodynamic model, input the streams information, and define the blocks operating conditions:

1. Click on the Components folder to expand it. You will see that there is a sheet named "Specifications" that needs to be filled. This sheet contains the component list that will

be used in the simulation. In here, you will input *all* components that are involved in the process. In our case we have water, acetone, and MIBK. Inputting components can be done by typing the component name directly or by searching for the component. If you type “water” into the Component ID column and hit enter, you will see that Aspen Plus immediately identifies that component and displays the rest of the information, which is already stored in its database. Similarly, typing “acetone” and hitting enter will include acetone in the list.

If you try to type “MIBK” and hit enter, Aspen Plus might not recognize the component and leave its name empty (newer versions might recognize this component). This is because Aspen Plus does not store MIBK with this name. Instead, it uses the full name. Therefore, we need to do a search on this component. To do so, select the row in which the MIBK has been entered and click the Find button. This will open the Find dialog as show in Figure 6.

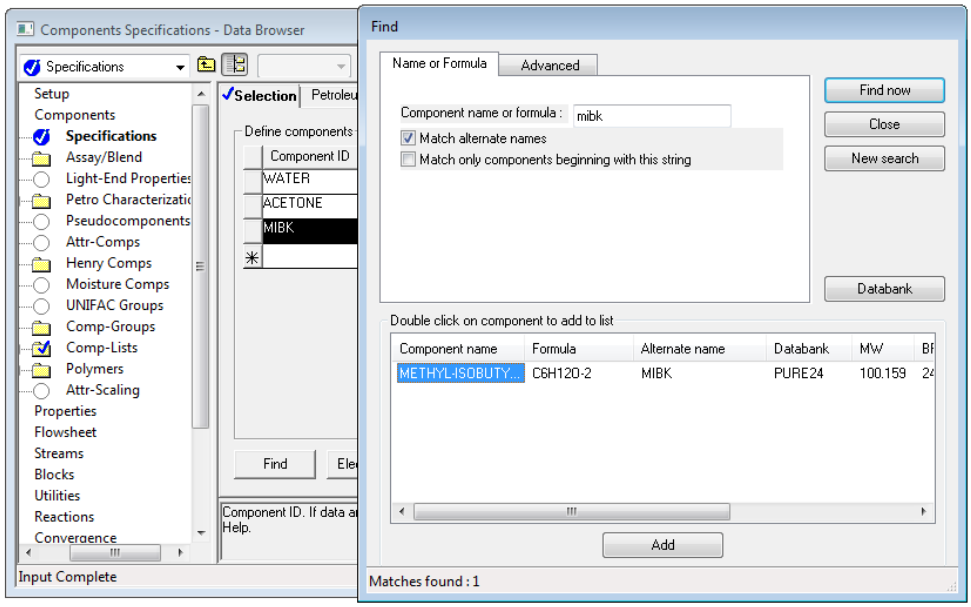


Figure 6. The Find dialog lets you search for components.

In the Find dialog, type MIBK and hit enter. You will see in the lower part a list of all matching components (in this case we have only one). After checking the formula and full name, we see that the $C_6H_{12}O$ is the one we are looking for. Select this component and hit Add.

Now we have added all the required components. Notice that the Specifications icon has changed to a circle with a check mark ( ) indicating that we have input at least one component successfully. You can continue add components if needed, but for this example we do not.

2. Next we go to the Properties folder. In this folder we can define the thermodynamic model to be used in this simulation. In addition we can define other properties related to the components chemistry and their transport properties. In this example, we will only deal with the thermodynamic model.

   To select a thermodynamic model, click on the Specifications sheet. Under the specifications sheet there are the "Property methods & models area" where you can select the model to be used for thermodynamic calculations. For this example, choose the NRTL method as the Base method. If the Parameters folder becomes highlighted with the red circle, click on it and on the highlighted form within this folder to confirm.
3. Now we can go to the streams folder to define the streams. Notice that in the streams folder only streams 1 and 2 are tagged as incomplete. The other streams are not. This is because streams 1 and 2 are inlet streams, thus they must be defined by the user as process variables. Streams 3, 4, and 5 are outlet streams and can be calculated, in principle, by the material and energy balances.

   Click on stream 1 and input the temperature, pressure, flow rate, and composition as shown in Figure 4, then click on stream 2 and do the same. After you have finished with all the information for streams 1 and 2, the streams folder should have the blue check icon indicating all information has been successfully entered.
4. Finally, we need to input the blocks information. What is meant by block information is the operating conditions or specifications at which the unit operation is operated or was designed, respectively. For an adiabatic mixer, as is the case here, we have one degree of freedom corresponding to the pressure drop across the mixer. Some blocks have default values so you do not have to worry about it every time, others do not. For the case of mixers, the pressure drop is set to zero by default. In general, it is good practice to check all blocks to make sure there everything makes sense.

   The other block, the decanter, must be also specified. The decanter works based on the phase behavior of the components (recall the extraction process calculations). Thus, we need to specify two operating conditions (two degree of freedom). In this case, we have to provide information about the operating pressure (or pressure drop) and the operating temperature (or heat duty). Based on the information given in Figure 4, we need to set the pressure drop to zero and temperature to 75^{o}F. The temperature specification is straight forward. The pressure drop, on the other hand, can be set by specifying zero absolute pressure. Whenever a pressure is set to zero absolute (for example, 0 psia) Aspen Plus interpret this as pressure drop. The specification sheet for the decanter should look as shown in Figure 7. Notice that not all information is required in this form. For example, the specification for "Key components to identify the 2nd liquid phase" is optional. By default, Aspen Plus uses densities to split the two liquid

phases. However, in some cases you might want to override this default which can be done using the "Key components specifications".

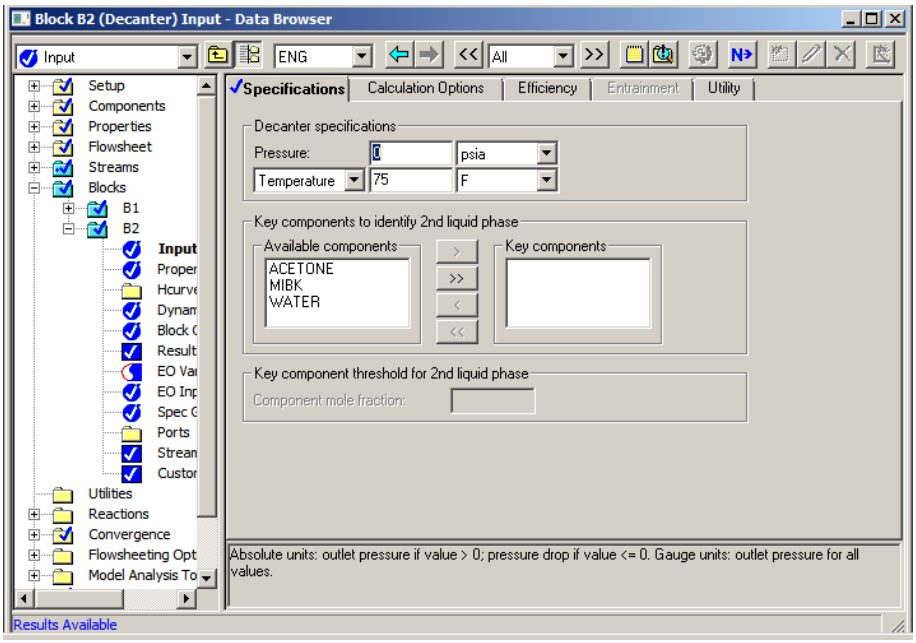


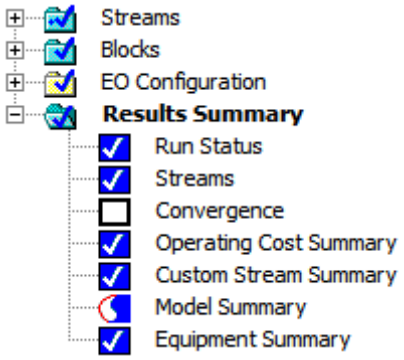
Figure 7. Specifictions for the decanter block in acetone removal process.

Now all the required information has been entered and the Status Bar message has changed to "Required Input Complete", indicating that we can run the simulation.

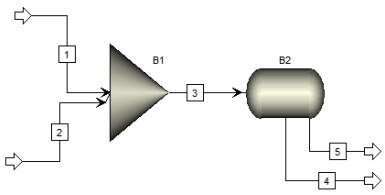
Running the Simulation and Viewing the Results

By running the simulation we mean performing the required calculations (material and energy balances, pressure drop calculations…etc.). To do so you can either hit the F5 key on your keyboard, click on the Start button ( ) on the Simulation Run toolbar, or select Run>Start from the Run menu. All will do the same function. Once you run the simulation you will see some visual indications of the calculations process in the flowsheet and the Status Bar message. If everything goes alright, the Status Bar will come up with the message "Results Available" indicating the calculations were successful. Now we are ready to view the results.

NOTE: *Successful Calculation* means that Aspen Plus was able to perform all numerical calculations with no mathematical errors. However, the only way to ensure that the results obtained are reasonable (or reliable, or realistic) is through making reasonable inputs and property method choices, good engineering judgment, past experience, and comparison to actual plant data. The general rule in using simulator tools is: Simulators are as good as the one who is using them, not more.



To view the results for each stream, you can double click on it to open the Data Browser for that stream. The dialog presented allows you to view the selected stream's properties and compare it with other streams if you wish. You can also view a summary of the results all together. To do so, notice that a new item (named "Results Summary") appears now in the left hand side of the navigation tree. The Streams sheet provides a convenient way of viewing all or part of the streams in the flowsheet. It also provides you with an option to create a stream table on the flowsheet (a common engineering practice). To create a stream table, just click on the Stream Table button on the Streams sheet. This will create a table with the stream indicated in the Streams sheet. By default, the Stream Table is quite big and contains more information than usually displayed in such tables. To modify the data viewed in the Stream Table, go to "Setup\Report Options\Stream" tab on the same dialog. A flowsheet with stream table is shown in Figure 8. Notice that you can control the appearance of the stream table by selecting its format in the Streams sheet.



Heat and Material Balance Table

Stream ID		1	2	3	4	5
Temperature	F	75.0	75.0	71.8	75.0	75.0
Pressure	psia	50.00	50.00	50.00	50.00	50.00
Vapor Frac		0.000	0.000	0.000	0.000	0.000
Mass Flow	lb/hr	100.000	100.000	200.000	103.042	96.958
Volume Flow	cuft/hr	2.003	1.610	3.550	1.679	1.924
Enthalpy	MMBtu/hr	-0.143	-0.682	-0.825	-0.677	-0.148
Density	lb/cuft	49.930	62.118	56.337	61.383	50.402
Mole Flow	lbmol/hr					
ACETONE		0.104		0.104	0.050	0.054
MIBK		0.938		0.938	0.021	0.917
WATER			5.551	5.551	5.443	0.107

Figure 8. Generating a stream table.

Another common practice in flowsheeting is to show the conditions of each stream on the flowsheet. This can be done by doing to "Tools\Options" and modified the options under the "Results View" tab. A flowsheet with temperature of each stream displayed on the stream is shown below.

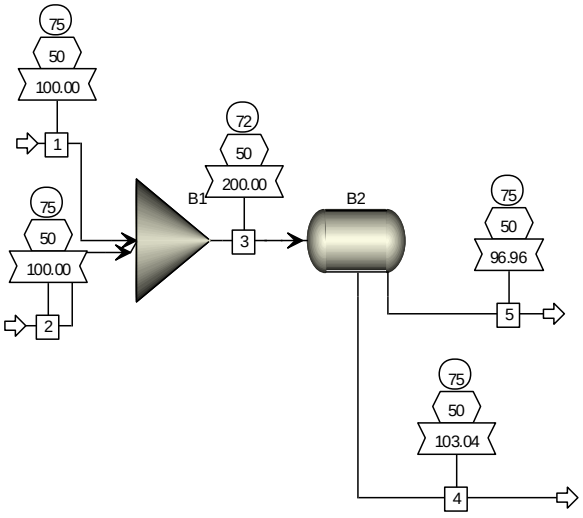


Figure 9. View results on streams.

Saving Your Project

It is a good practice to save your work frequently to avoid unexpected loss. You can save your project using the File>Save… menu (or using the Save As window if you would like to change the file name or extension). By default, the file extension for saving Aspen Plus projects is apw (short for Aspen Plus Worksheet) with the icon shown to the right (called the Aspen Leaf logo).

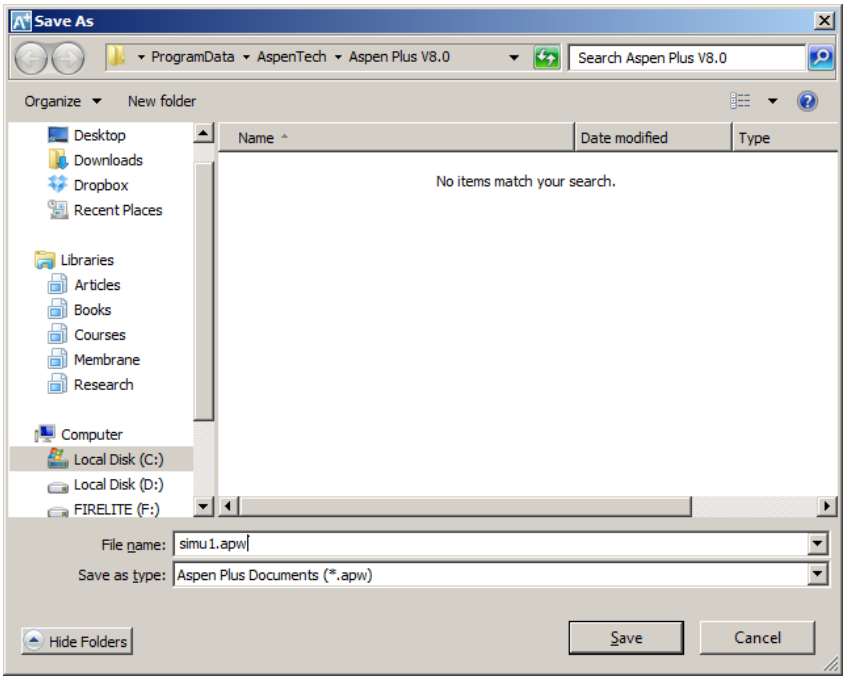


Figure 10. Saving window dialog in Aspen Plus.

The apw format is one of several formats that can be used for saving a project. The other formats being bkp (backup file), apwz (compound file), and apt (template file). When saving as an apw file, all input, results, and intermediate convergence (calculations) information are saved. Thus, the next time you open an apw file it will look exactly as when you closed it. On the other hand, saving as a bkp file only saves the input information and results output. Therefore, apw files are typically larger than bkp.

If you save your file to a folder, say the Desktop folder, you will also notice that other files in addition to apw and bkp have been created by Aspen Plus. These are files that is used internally by Aspen Plus to record the input and output data. Table 1 shows the major formats that you might encounter when saving an Aspen Plus project. Generally, the apw or bkp file is sufficient to be able to open the project on other machines.

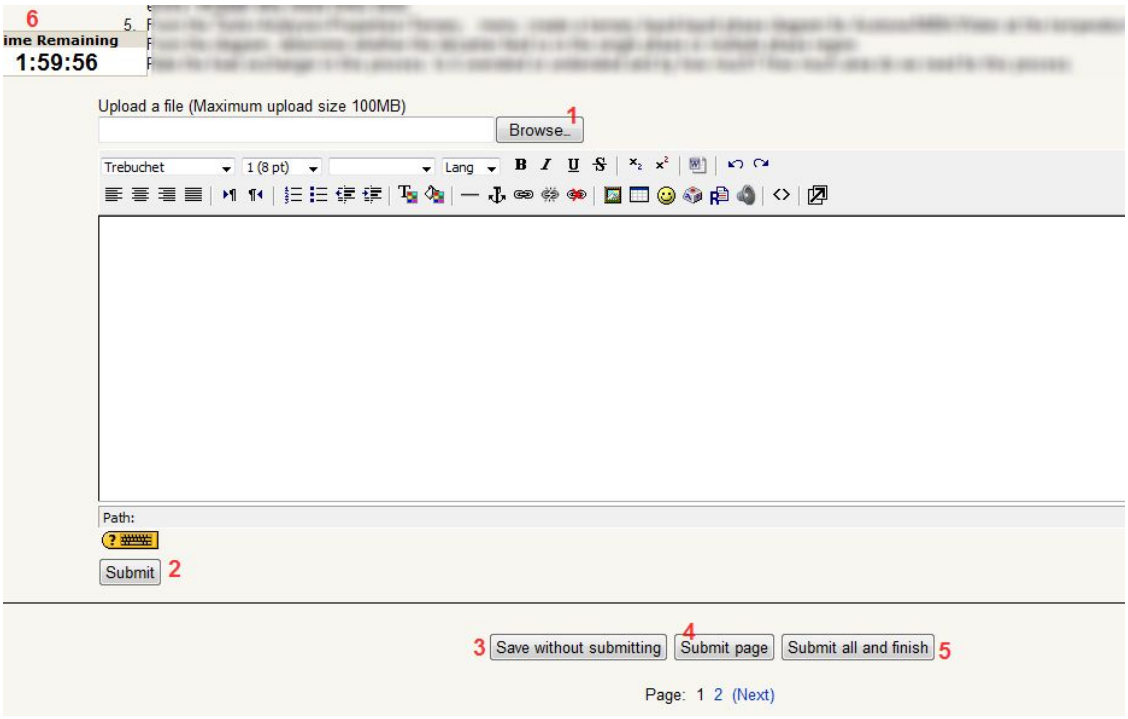
Table 1. Major types of file formats used by Aspen Plus. For more information see "File Formats in Aspen Plus" in Aspen Plus Help.

File Type	Extension	Format	Description
Document	*.apw	Binary	Quick restart file containing simulation input and results and immediate convergence information
Compound File	*.apwz	Binary	Consolidated file containing all files used by a simulation
Backup	*.bkp	ASCII	Archive file containing simulation input and results.
Template	*.apt	ASCII	Template containing default inputs
Input	*.inp	Text	Simulation input
Run Message	*.cpm	Text	Calculation history shown in the Control Panel
History	*.his	Text	Detailed calculation history and diagnostic messages
Summary	*.sum	ASCII	Simulation results
Problem Definition	*.appdf	Binary	Binary file containing arrays and intermediate convergence information used in the simulation calculations
Report	*.rep	Text	Simulation report
Model Library	*.apm	Binary	User-created model library consisting of pre-configured models or flowsheets for distribution and re-use.
Embedded Backup File	*.apmbd	Binary	Information on objects such as spreadsheets and pictures embedded in the Aspen Plus simulation
DFMS file	*.dfm	Text	Parameter values used in a simulation, or prepared as input for a user databank
Project data file	*.apprj	Text	Parameters values used in a simulation in the form of Prop-Data input language

Submitting Your File Using JUST Elearning

During this lab you will be asked to submit your simulation using the elearning page of the course. It will be your responsibility to submit the correct file correctly. Below are the steps to do so:

1. Save your project using the apw extension. Your file name should be in the following format: ID#_Quiz#.apw. For example, if your student ID number is 20060022001, and you are saving the file for quiz 1, then your file name should be 20060022001_Quiz1.apw. To make it easier to find the file, create a folder (call it Aspen) on the desktop and save all your projects in this folder.
2. Go to the quiz page on the elearning site. In this page, select the Browse button (1 in the figure below) and navigate to the folder where you saved your project, then click OK.

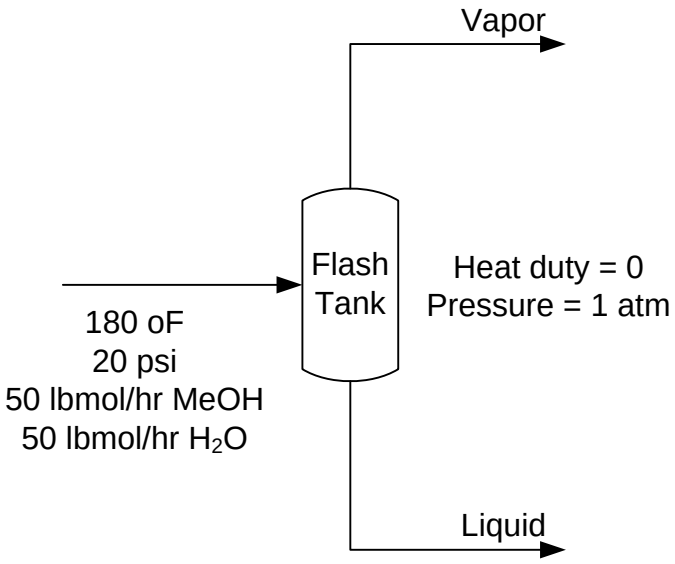


3. To upload your file you can either click:
    a. Submit (2): this will upload the file but you can still work on the quiz if needed. If you decided you have uploaded the wrong file, you can repeat the upload process again and click Submit. Clicking Submit will let the instructor see your work but he will not be able to grade it.
    b. Save without submitting (3): this will upload the file but will not send the file to the instructor.
    c. Submit page (4): this is equivalent to Submit except that it will submit all questions in the page.

d. Submit all and finish (5): this will upload your file and submit the quiz for grading. Generally, you will not be able to work on the quiz after you click this button. You must click this button when you are finished in order to get a grade for the quiz.

Exercise 1:

Simulate the following flash tank with the NTRL model.

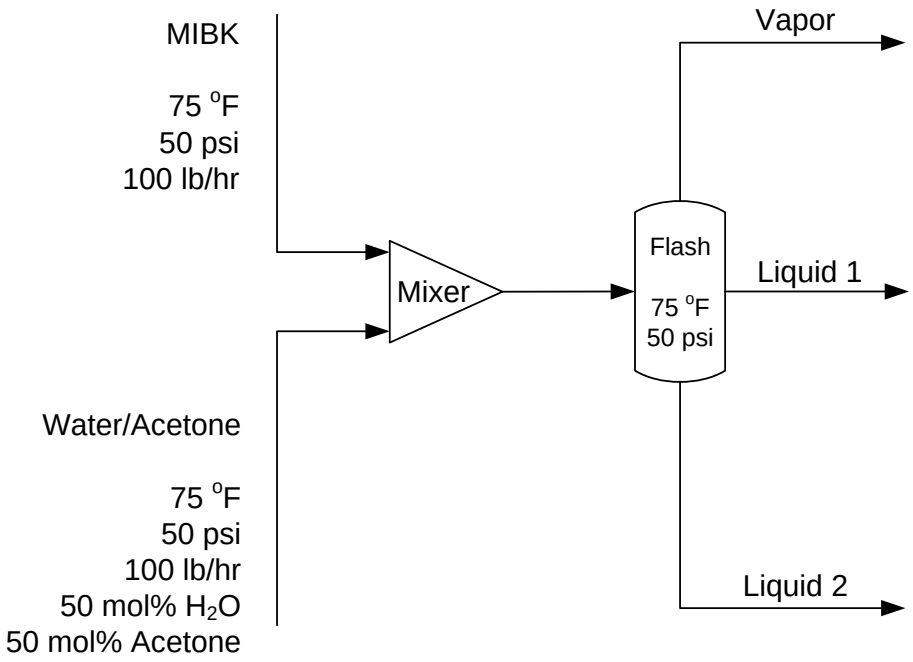


Questions:

1. What are the mole fractions of MeOH in the vapor and liquid output streams?
   Vapor _____ Liquid _____
2. Change the property method to "IDEAL", rerun the simulation. What the mole fractions of MeOH now?
   Vapor _____ Liquid _____
3. Try to prepare the simulation for print by experimenting with the Page Break Preview option under the View menu.
4. As a tool for double checking someone's work, it is sometimes useful to check all the inputs made by the user. For example, a supervisor with more experience about the process might want to check the work of a new engineer to avoid input mistakes or bad assumptions. Generate an input summary file from the View menu and look at its content.

Exercise 2:

Simulate the following extraction process using the SRK property method.



Questions

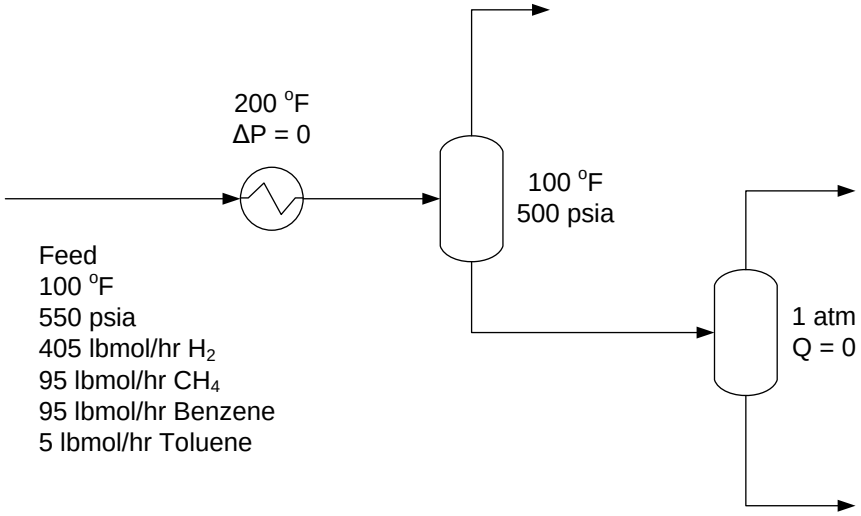
1. Generate a stream table for the inlet stream of the flash and the three output streams. How much acetone was picked up by the MIBK? _____
2. Compare the total flow rate and fraction of acetone in the Liquid 2 stream using the following property methods:

Property Method	**Flow rate [ ]**	**Acetone % [ ]**
RK-Soave		
IDEAL		
Wilson		
NTRL		

Study the results and see what the differences between the models are.

Exercise 3:

Build a simple flowsheet to purify a benzene containing mixture using a series of simple flash drums. The flowsheet is shown below. Use Peng-Robinson property method and the conditions shown below.



Questions:

1. How much of the hydrogen and methane was removed from the final product?

2. What is the mole fraction of benzene in the final product?
3. How much benzene and toluene were lost as vapor?
4. What is the ratio of benzene to toluene in each stream?

5. Make a case study on the effect of the heat exchanger temperature, and first flash pressure on the benzene mole fraction of the final product:

Temperature	Ben. mol frac.

Pressure	Ben. mol frac.