Introduction to ASPEN Simulation
Bubble Point, Dew Point and Flash Calculations

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In this exercise you will simulate several flash processes and calculate bubble and dew point temperatures for a process stream using a chemical process simulation package from Aspentech. This tutorial is designed for new users of ASPEN

Instructional Objectives

1. Change the default set of units
2. Select chemical species
3. Use the Peng-Robinson Thermodynamics package.
4. Install a simple flash drum separator
5. Specify input stream variables of temperature, pressure, flowrate and composition.

This program is used by industry to design and simulate process plants such as oil and gas refineries, chemical and pharmaceuticals production facilities. According to their website[1]

- 800 Universities worldwide
- 32 of the top 32 petroleum companies
- 50 of the top 50 chemical companies
- 19 of the top 20 pharmaceutical companies
- 17 of the top 20 engineering & construction companies

For more information on Aspentech go to http://www.aspentech.com

The overall process for this simulation is to

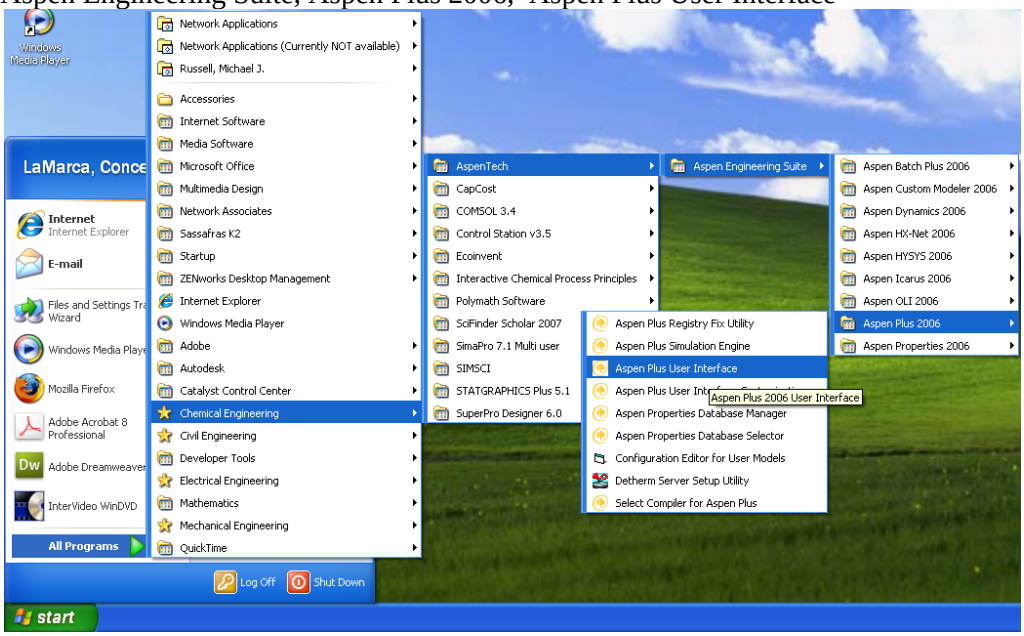
- Setup the system of units that will be used in the simulation (you will use a modified metric system)
- Select Chemical Components: *i*-Pentane, *n*-Pentane, and *n*-Hexane.
- Select a thermodynamics package that describes the physical and chemical properties of the chosen chemicals – Peng-Robinson Equation of State.
- Select the unit operations (Flash Drum Separator)
- Define all required inputs and 2 variables in the drum.
- Run the program and examine the results

Rowan University has a license to run Aspen Plus 2006 – aspenONE.

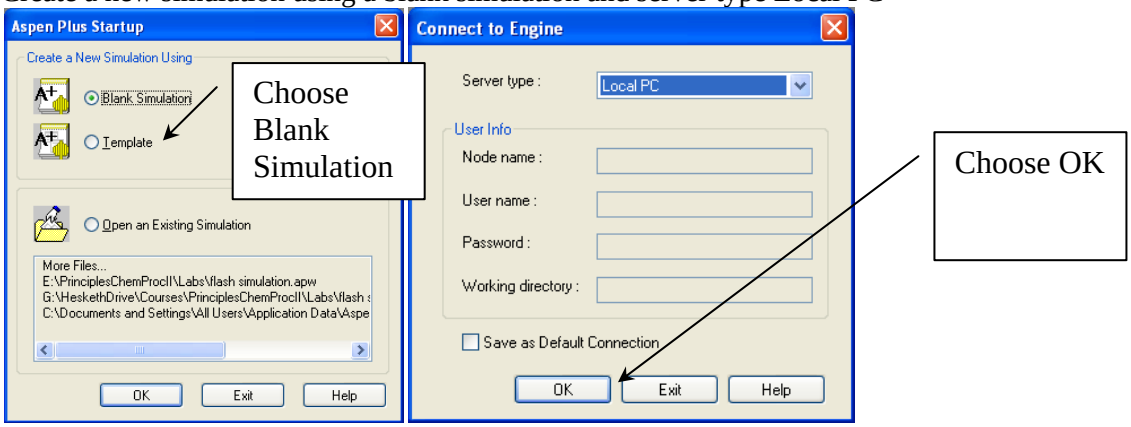
[1] Aspentech Website, http://www.aspentech.com/corporate/university/index.cfm

Procedure to Create a Flash Separation Model:

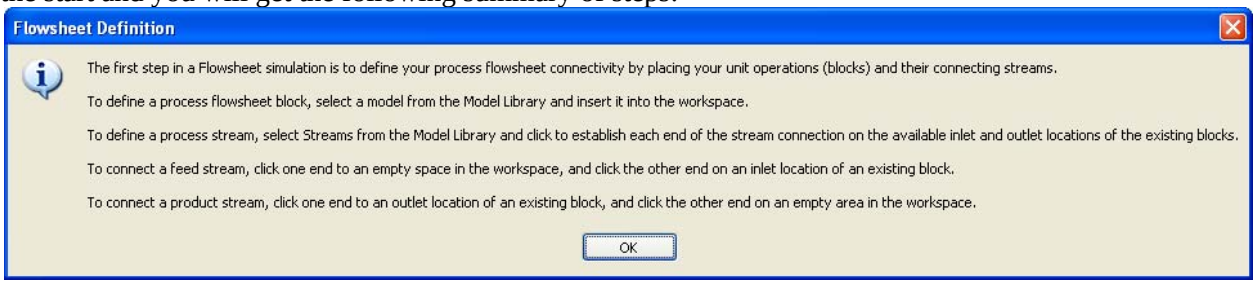
1. Start Aspen Plus User Interface by going through the start menu, Chemical Engineering, AspenTech, Aspen Engineering Suite, Aspen Plus 2006, Aspen Plus User Interface



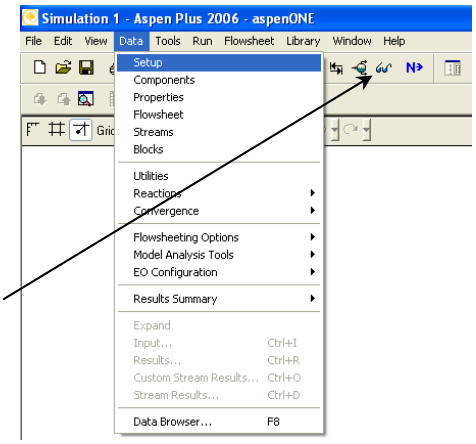
2. Create a new simulation using a blank simulation and server type Local PC



3. One way to proceed through the setup screens is to click  to take you to next action. Do this at the start and you will get the following summary of steps:

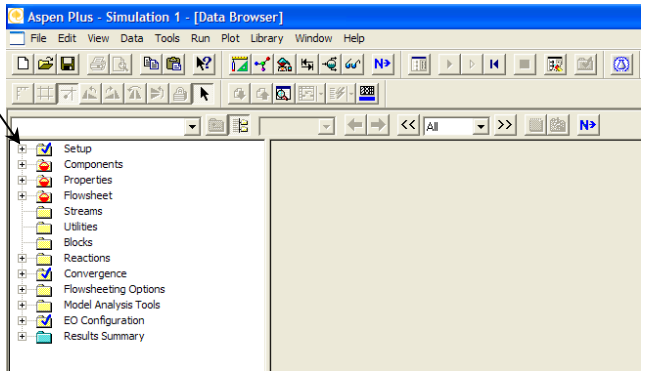


4. Choose *Data, Setup* from the main menu or use *Data Browser* from the eyeglass icon, and select Setup.

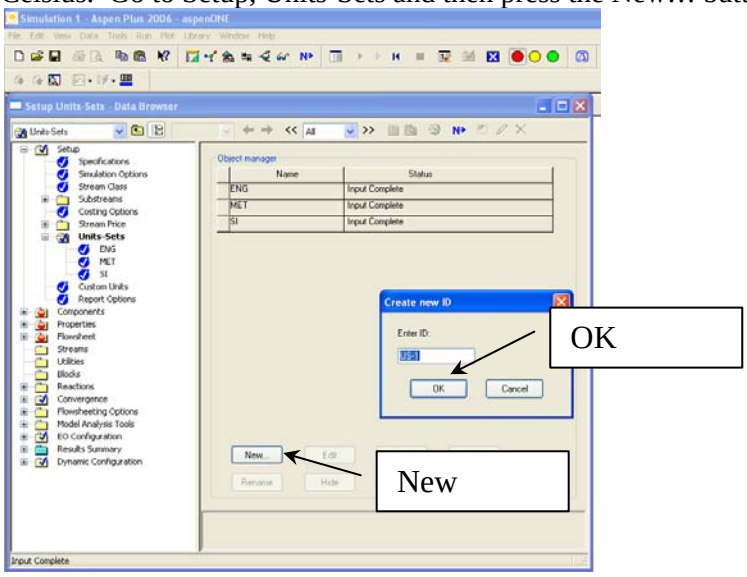


Eyeglass Icon

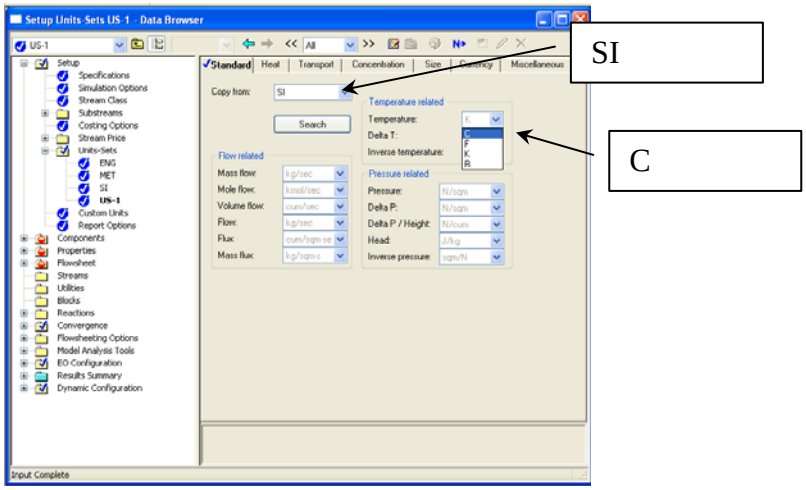
Data Setup



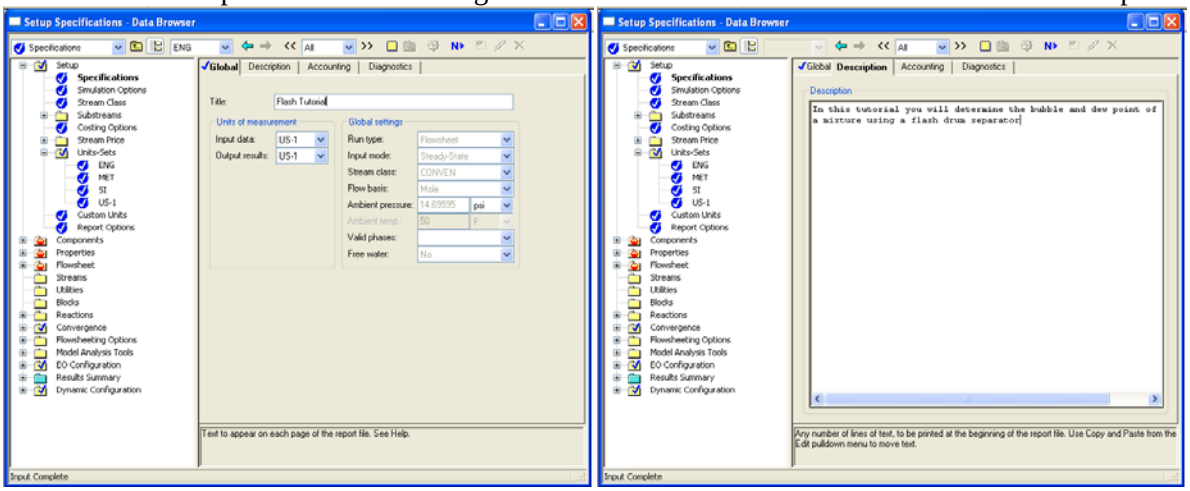
5. We will now define a unique unit set that is in the metric system with units of Temperature of Celsius. Go to Setup, Units-Sets and then press the New… button.



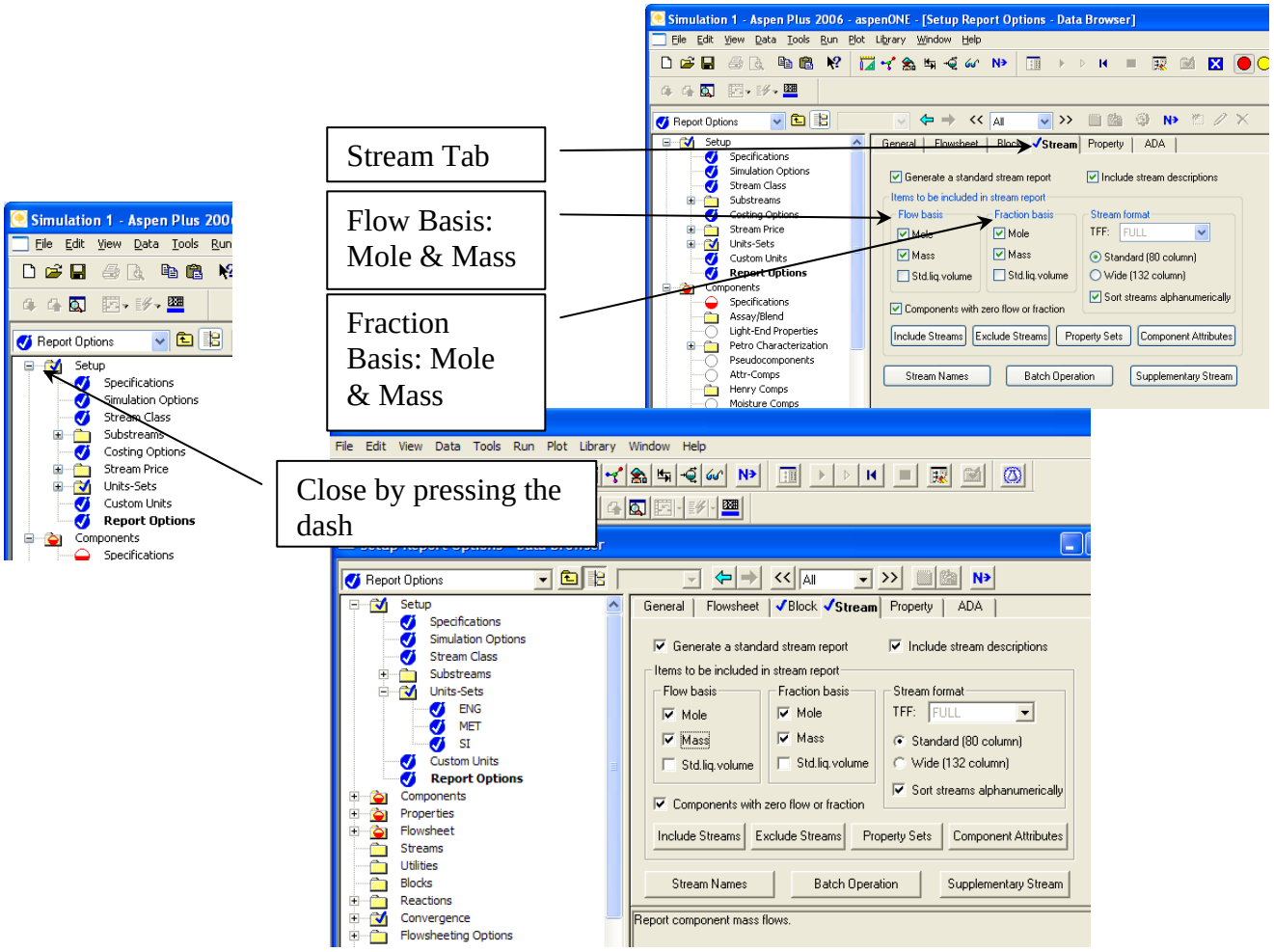
6. Choose SI and C for Celsius. You can always go back and adjust the units to what you would like them to be.



7. Go back to Specifications and give this tutorial a title and add a description.

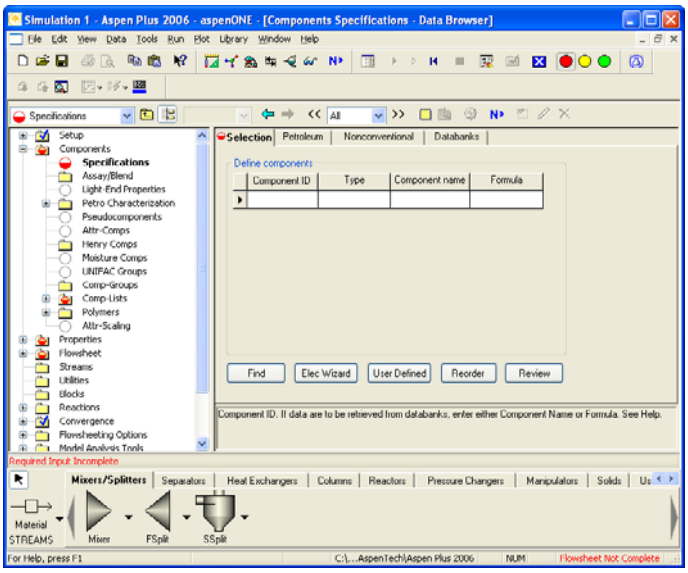


8. Before proceeding, move to *Report Options* where you can specify the information that will be printed in a final report. Under the *Stream* tab, select both mole and mass in the flow basis field as well as the fraction basis field. Close the *Setup* section by pressing the dash in the box next to setup.

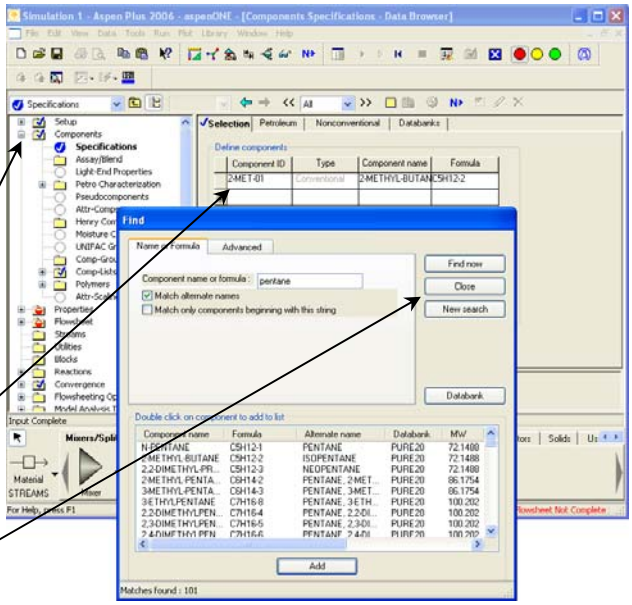


9. Click  to take you to next Input step. Using the Next button will help guide you to each step that needs to be performed.

10. If you didn't click next then, choose the *Components* option in the data browser window to start adding chemical components, and select *Specifications*.



11. Next select the chemicals for your reaction system. Use the *Find* button to search for the components for this problem: *i*-Pentane, *n*-Pentane, and *n*-Hexane. Select your component from the list, and then *Add* it. When finished, close the *Components* section.

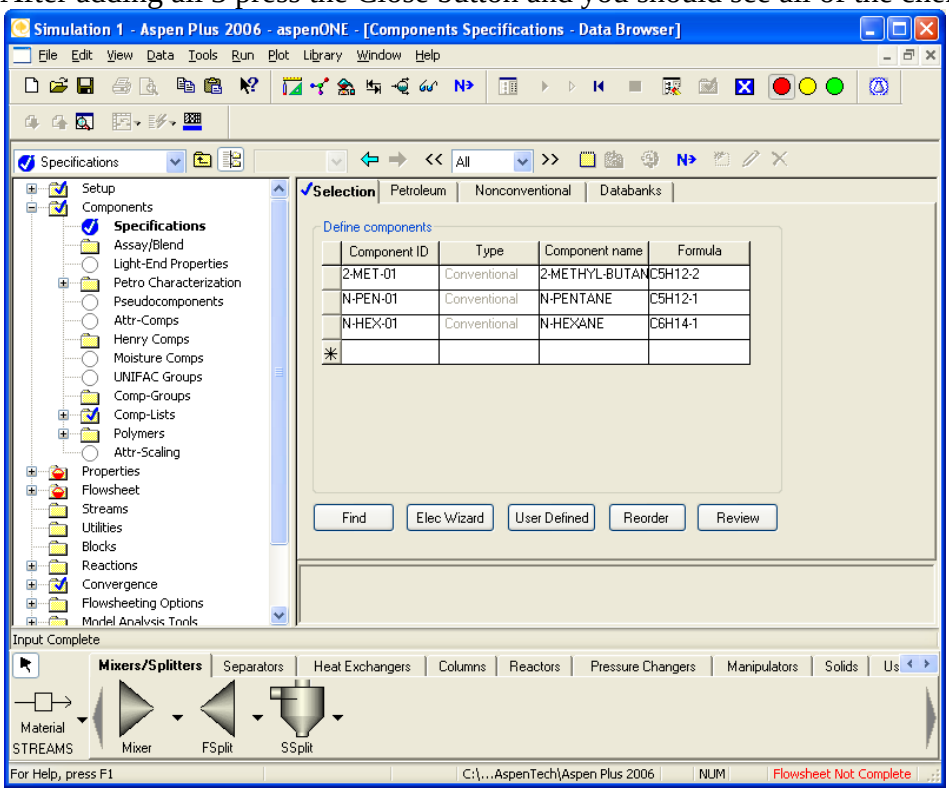


Close by pressing the dash

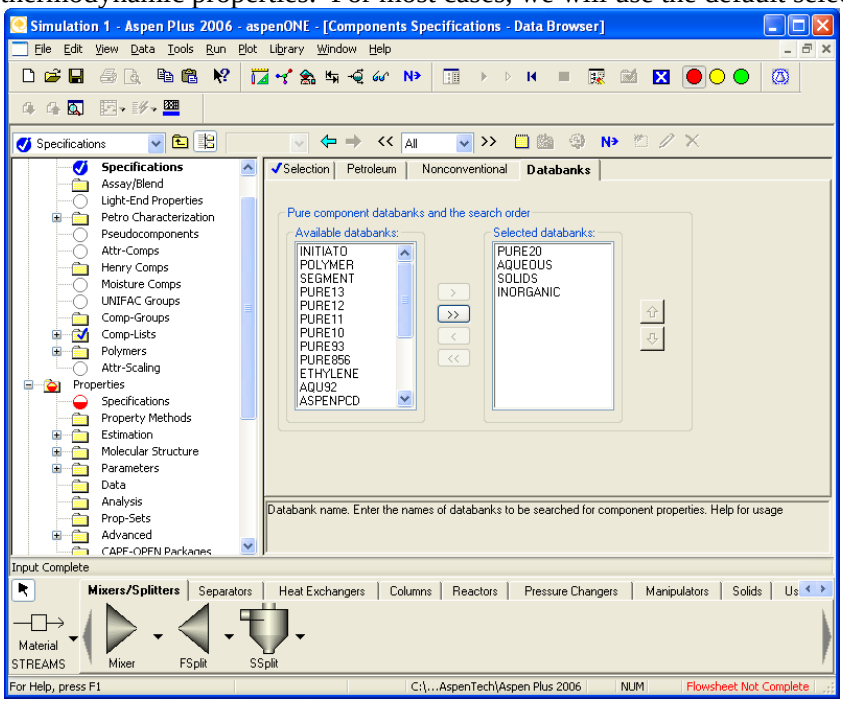
After pressing the Add button the chemical appears it appears here

After adding all 3 chemical species press the Close button

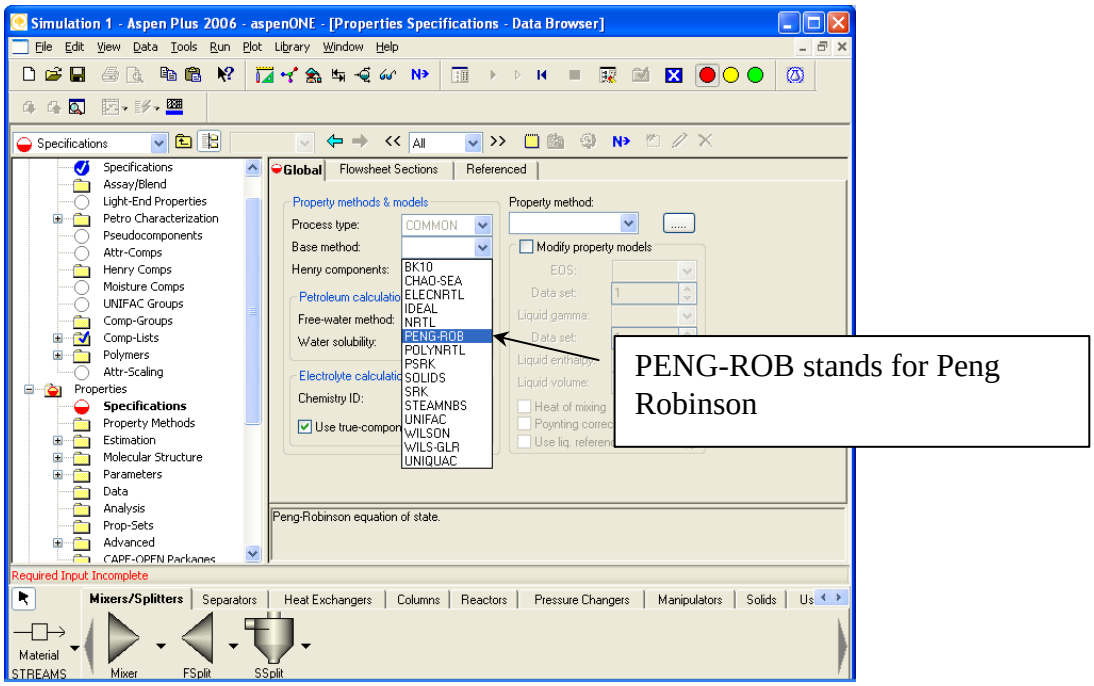
12. After adding all 3 press the Close button and you should see all of the chemical components



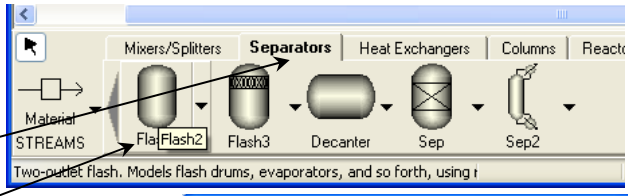
13. The *Databanks* tab shows the preferred databanks from which Aspen will draw physical and thermodynamic properties. For most cases, we will use the default selection.



14. Next, select as base method for system properties, by selecting *Properties, Specifications*. Since these compounds are hydrocarbons, use the Peng-Robinson thermodynamics package by selecting PENG-ROB under the *Base method* tab. This is an equation of state that is excellent for hydrocarbon components. You will learn more about this in your chemical thermodynamics classes. Close the *Properties* section and the *Data Browser* (and all other windows) revealing the blank Process Flow Window.



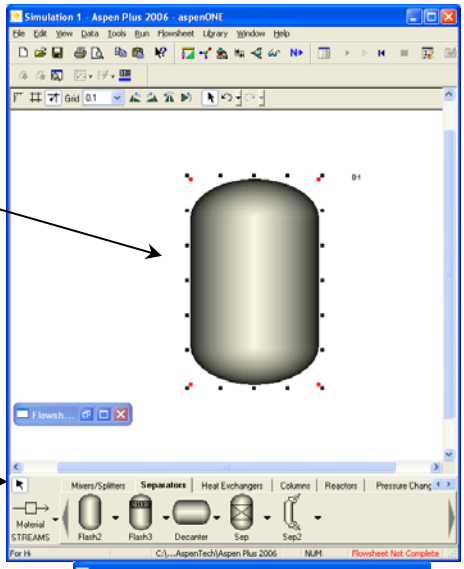
15. You are now ready to setup your flowsheet. You should see the blank Process Flow Window. You will now create a flash simulation by adding the equipment that will separate a vapor and a liquid. This equipment is called a flash drum. Click on the separator tab and you will see a number of separators.



Click Separator Tab

Click once on Flash2 and release

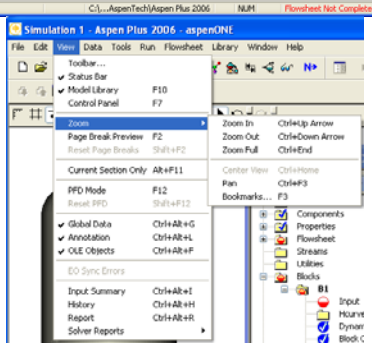
Move cursor to PFD section (you will see a black cross)



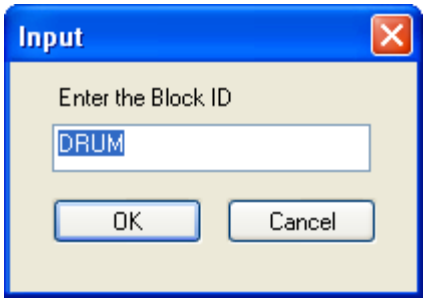
16. Click with the left mouse button on Flash Drum 2 and then release the left mouse button. Next move cursor onto the Process Flow Window and then press left mouse button only once. Select the arrow in the very left corner of the model library taskbar.

To finish adding equipment press this arrow

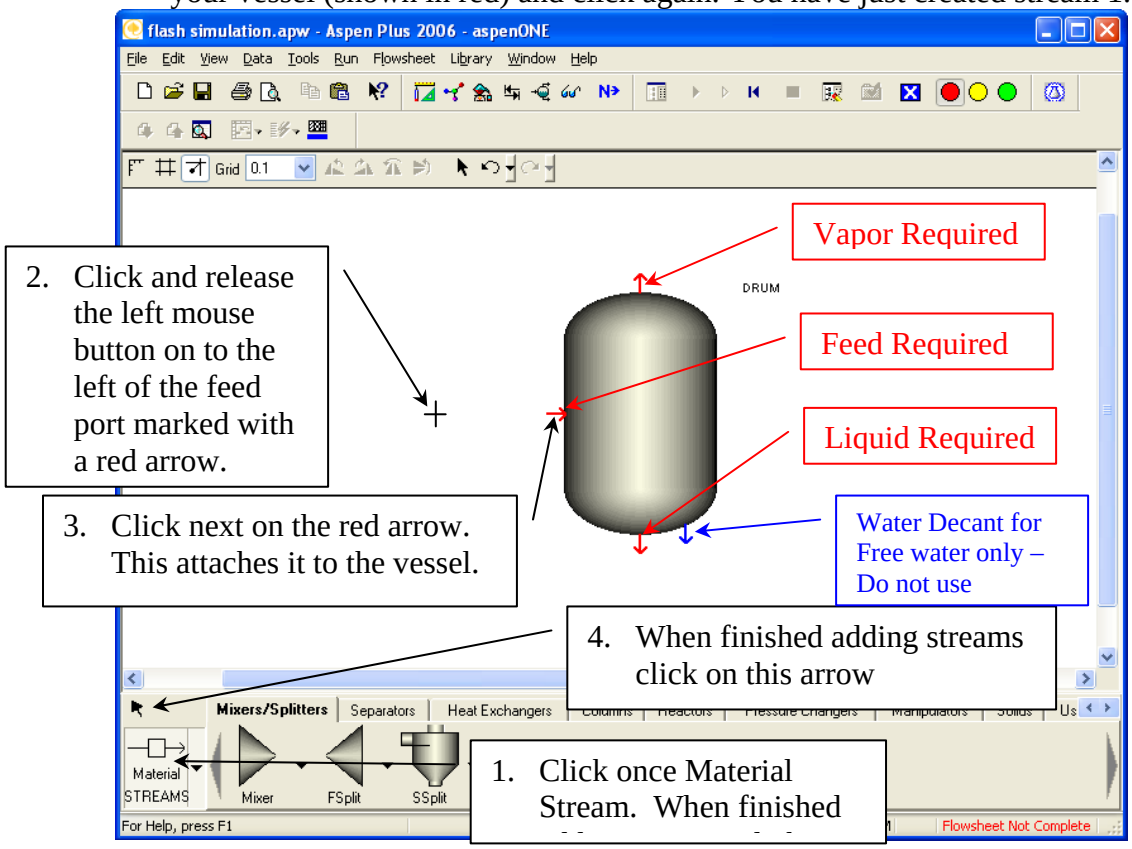
17. To see a larger image go to the view menu and adjust the size. Pan will center the drum in the pfd.

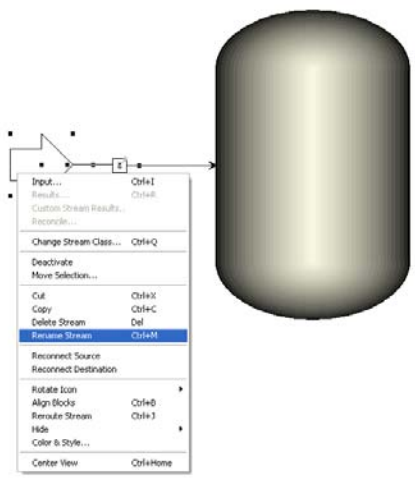


18. Rename the separator using a descriptive name by right clicking and selecting *Rename Block.*

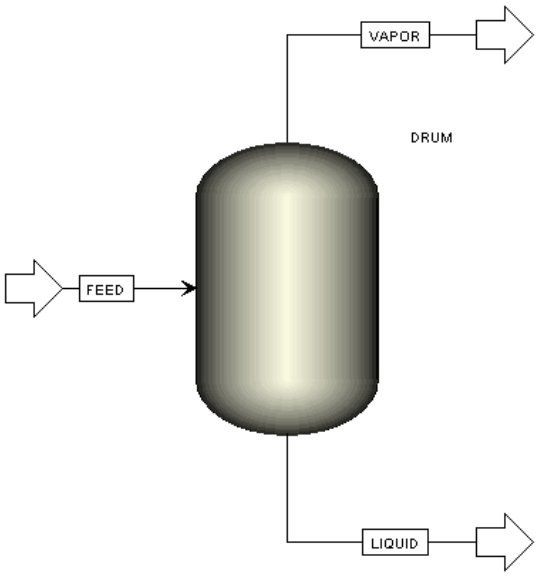


19. To add feed and effluent streams, use the *Model Library* to select the *Material STREAMS* tab in the lower left-hand corner and click once. This will allow you to place multiple streams as needed. Move the cursor, now a crosshair, onto the process flowsheet. Notice that ports on the flash drum are either red or blue. Ports that must have at least one stream connected are shown in red. Other optional ports are shown in blue. If you position the mouse over a displayed port, the arrow is highlighted and a text box with the description of the port appears. Click once, drag the cursor to connect the first stream to the feed port of your vessel (shown in red) and click again. You have just created stream 1.



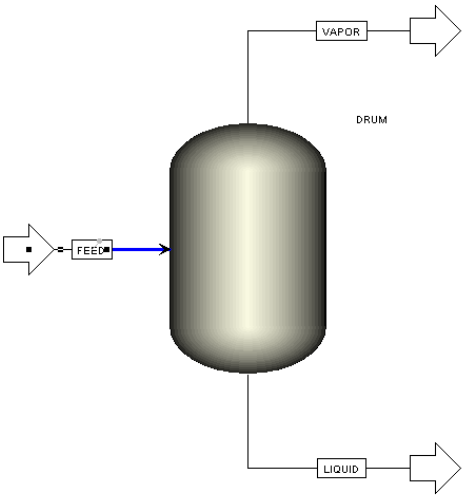


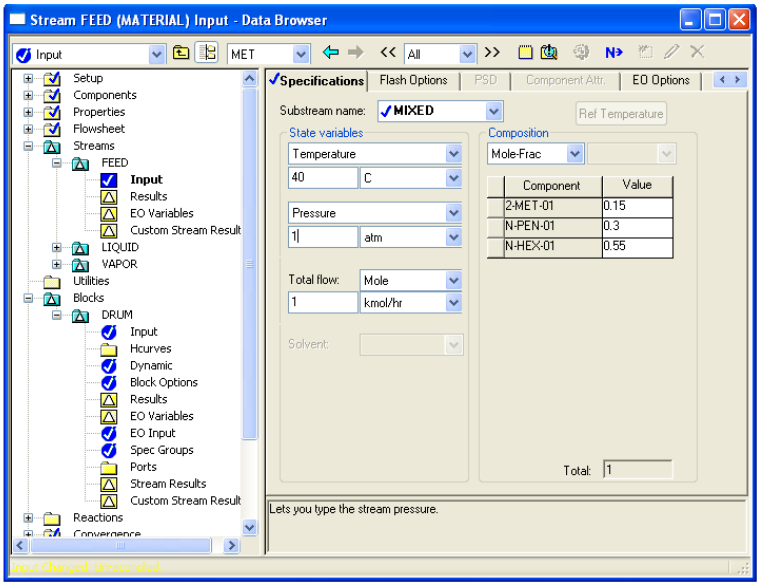
20. Add two outlet streams to the flash drum in a similar way. (To modify your stream connections, select the small arrow, right click on the stream in question as select *Reconnect Source* or *Reconnect Destination.* Rename streams by right clicking on them so that you have a Feed, Vapor and Liquid Stream.



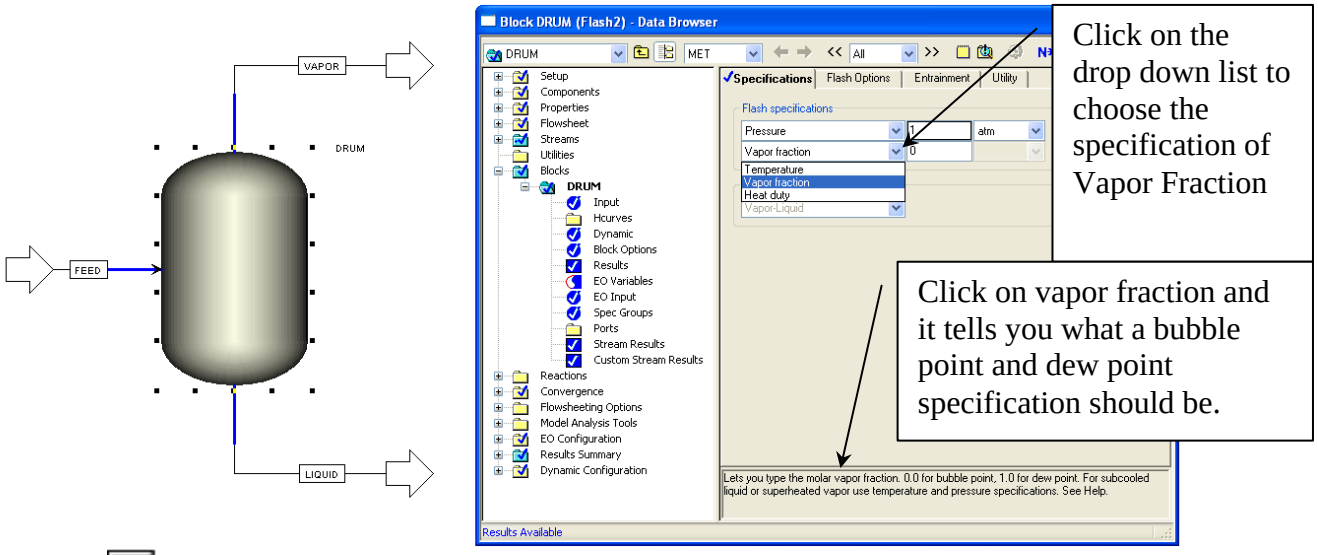
21. Specify the conditions of the feed stream (Double click on the stream or right click on it and then choose input). The inlet pressure is P= 1 atm, T=40°C, and the Feed stream total flowrate is 1 kmol/hr

Species	Mole Fraction
i-pentane	0.15
n-pentane	0.3
n-hexane	0.55

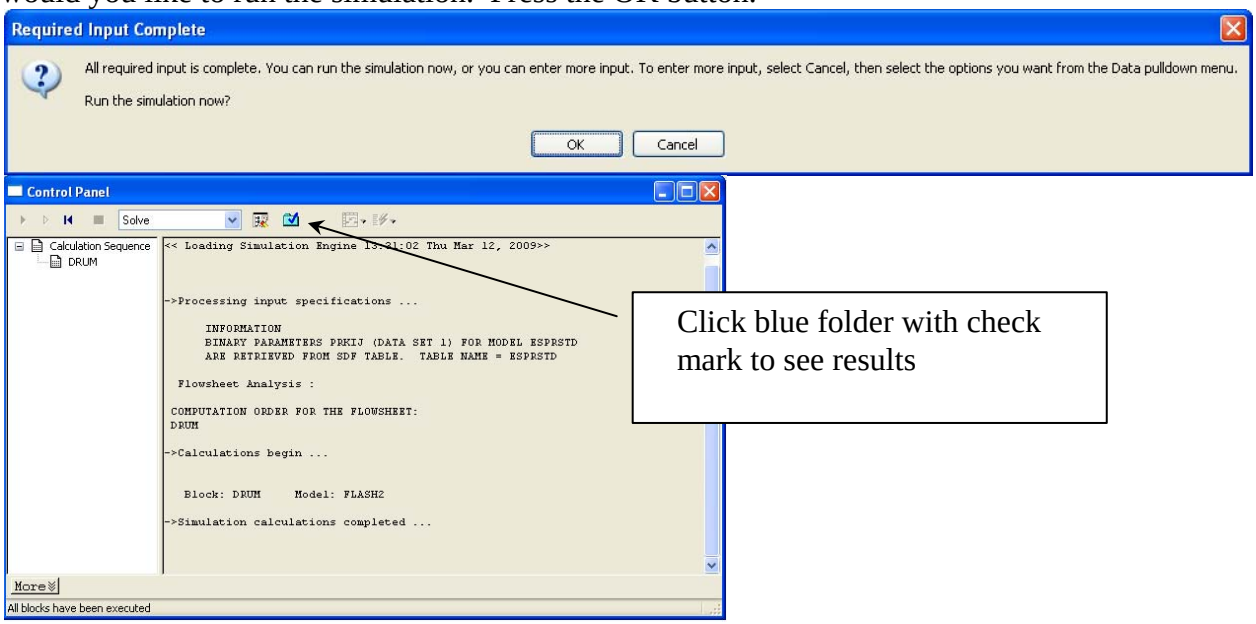




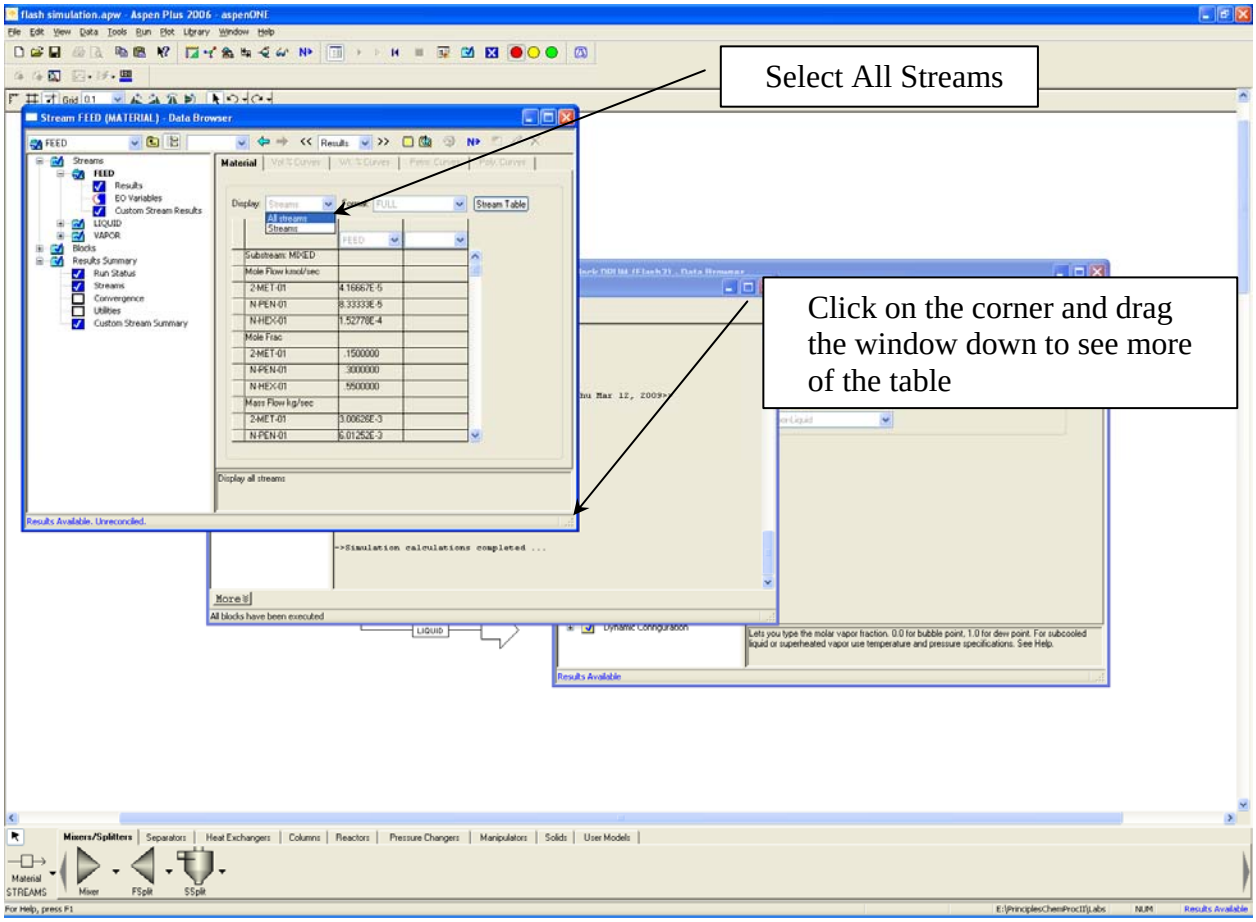
22. Now specify 2 variables for the flash drum. One of these variables will be the pressure in the drum which is at 1 atm. To do this either double click on the drum or press the button. For your first calculation you would like to determine the bubble point temperature at 1 atm. To do this you will set one of the 2 specification to give a vapor fraction is 0.0. Next determine the dew point.



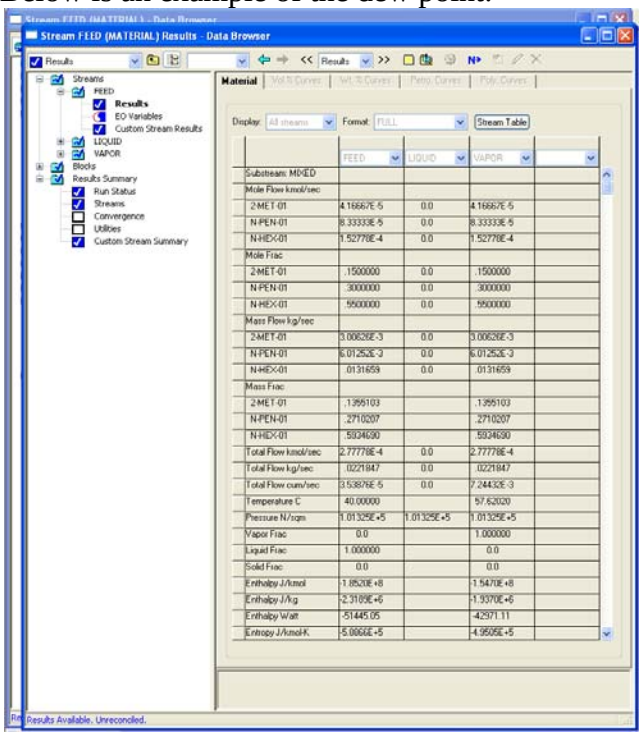
23. Press the button and it should give you a pop up screen that everything is complete and would you like to run the simulation. Press the OK button.



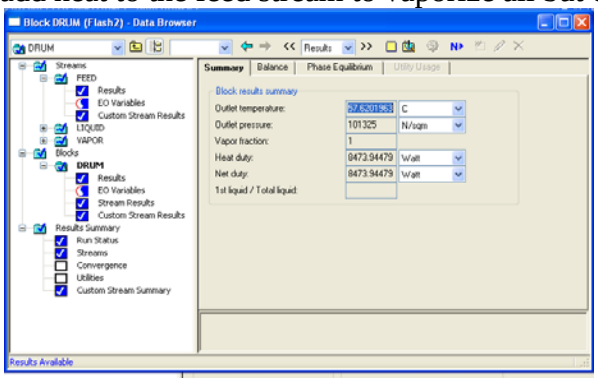
24. You have now performed your first ASPEN simulation! Now you need to look at the results. Click on the blue folder with a check mark  on it to see the results. First examine the feed stream to check to see what was entered.



Below is an example of the dew point:



Below is an example of the Drum Specifications at the Dew Point. Notice that you needed to add heat to the feed stream to vaporize all but one drop of fluid!



25. Run both the dewpoint and the bubble point and give the following:
Dewpoint temperature= _ _____**Bubble point temperature** =_____

26. Save the file on your galaxy drive. File, Save as, and change the path to your personal galaxy drive. I would suggest always saving your files with a unique descriptor (your name). The files are always printed with your filename showing on the page.

27. Now you have learned the how to use a tool that can give you an unlimited number of practice problems for hand calculations. Perform a hand calculation to determine the heat duty on this flash drum. As inputs use the flowrates, mole fractions and temperatures given in this simulation. **Calculate the heat duty for a case in which both gas and liquid are formed in the flash drum and the molar vapor fraction formed from the feed is between 0.2 and 0.8**. (Notice the heat duty is given in the Blocks, DRUM shown above). Since Felder did not give the heat capacities for all of the chemical I have given you a set below.

$$C_p = CPVAPA + CPVAPB * T + CAVAPC * T^2 + CAVAPD * T^3$$

The units of heat capacity are in cal/(mol K) and the units of temperature are in **KELVIN**

Table 1: Ideal Gas Heat Capacity Constants and heat of Vaporization.[i]

Species	*CPVAPA* *(cal/mol K)*	*CPVAPB* *(cal/mol K^2)*	*CPVAPC* *(cal/mol K^3)*	*CPVAPD* *(cal/mol K^4)*	T_{bp} *(K)*	ΔH^{vap} at T_{bp} (cal/mol)
i-pentane	-2.275	1.210E-1	-6.519E-5	1.367E-8	301.0	5900
n-pentane	-0.866	1.164E-1	-6.163E-5	1.267E-8	309.2	6160
n-hexane	-1.054	1.390E-1	-7.449E-5	1.551E-8	341.9	6896

28. To create a report file for the case you will perform a hand calculation of the heat duty for printing, select the File menu & Export. Under the Export screen choose Report Files (*.rep) as your file type and save.

At the end of this exercise submit a printout of the following:

- **Submit on Blackboard two aspen files:**
  - filename.apw (the case file for running Aspen)
  - and the report file filename.rep. This file should contain the case for your hand calculation.
- **Submit the hand calculations for the next homework session.**

[i] Reid, R. C., J. M. Prausnitz, T. K. Sherwood, "The Properties of Gases and Liquids," 3rd ed., McGraw-Hill 1977.