ASPEN Steam Table and Simple Heater Simulation

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In this exercise you will use a steam table thermodynamics package in ASPEN to simulate the heating and mixing of 2 input streams containing only water. This exercise will also introduce you to the concept of specifying an outlet condition and solving for an inlet condition. This tutorial is suitable for new users of ASPEN that have the ability to solve problems given in the chapter on energy balances (Chapter 7) of Felder and Rousseau[1].

Instructional Objectives: By completing this tutorial you will be able to

1. Change and use the default set of units
2. Select chemical species
3. Use a steam table thermodynamics package.
4. Install a simple heater
5. Fully specify the variables of temperature, pressure, flowrate and composition for a feed stream and for a heater the heat duty and pressure to calculate the outlet stream properties.
6. Specify all but one of the feed stream variables (e.g. temperature), the heat duty and pressure drop in the heater, and specify an outlet stream variable such as temperature. With these specifications use the Flowsheeting Options, Design Spec to calculate the temperature of a feed stream given the outlet stream temperature specification.

You will perform a hand calculation and simulation for all of the cases given below.

Case 1 a&b: Feed Fully Specified

Two feed streams and one outlet stream are connected to a heater. The first feed stream contains liquid water at 100°C and 10 Bar and has a mass flowrate of 2 kg/s. The second feed stream contains saturated steam (water vapor) at 8 Bar and a flowrate of 1 kg/s. The outlet stream is also at 8 bar. Determine the outlet temperature of the stream if

a. **The heater were adiabatic (heater acting as a mixer)**
b. **The Heat Duty of the heater is 8400 kJ/s. (The heater is adding 8,400 kJ/s to the fluid streams)**

Perform these 2 hand calculations to determine the temperature of the outlet stream for both cases using the steam tables in your text. After completing these hand calculations follow the steps given below to perform a simulation.

Case 2: Feed not fully specified

For the second simulation, instead of specifying the temperature of stream 2 you will specify the outlet temperature of stream 3. For this simulation you have been requested to achieve a temperature in stream 3 of 700°C at 8 bar using a lower heat duty than in case 1b on the heater of 7236 kJ/s. You have the same feed stream 1 at 100°C and 10 Bar and a mass flowrate of 2 kg/s. For this problem you must determine the temperature of the second feed stream which will be at a new pressure of 10 Bar and mass flow rate of 1 kg/s.

[1] *Elementary Principles of Chemical Processes of Chemical Processes Student Workbook*, 2005 Ed, R.M. Felder, R.W. Rousseau, G.S. Huvard, John Wiley & Sons, 2005.

This problem will be more difficult for ASPEN since it solves each unit operation (block) in a sequential manner. It always takes the input streams and input specifications and solves for the output conditions. In this case we will install a Design Specification operation from the Flowsheeting options. You will provide an initial guess and ASPEN will iterate using a convergence method to solve the system of equations until it finds a suitable answer.

Before proceeding you must have performed 3 hand calculations.

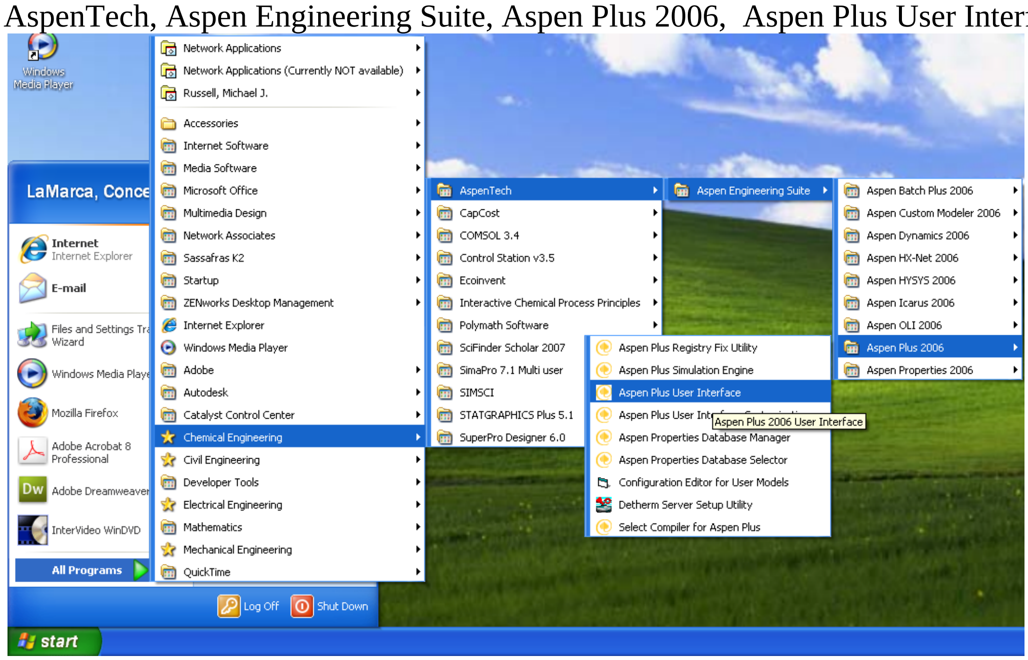
Case 1a	T3=
Case 1b	T3=
Case 2	T2=

Next follow the steps given to perform a simulation.
The overall process for the first simulation is the following:

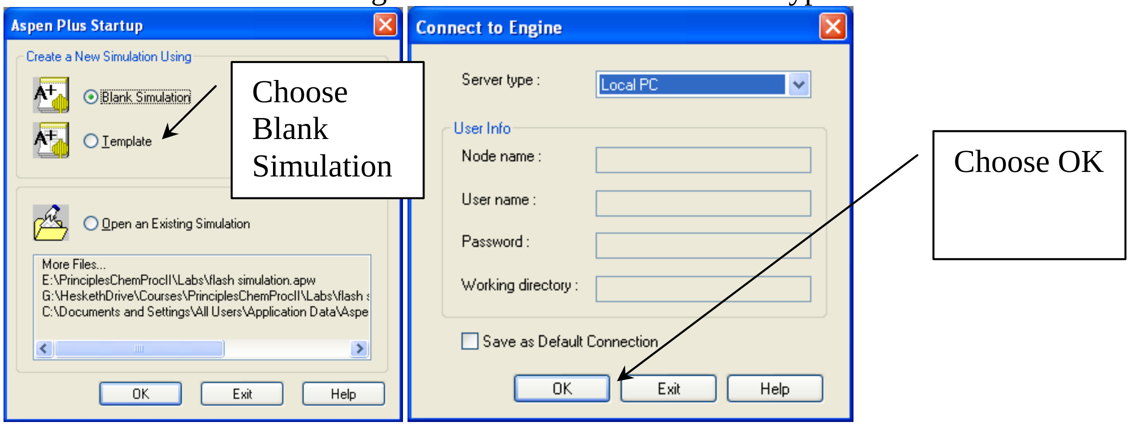
- Setup the system of units that will be used in the simulation (you will use a modified metric system)
- Select the chemical component for this simulation: water
- Select a thermodynamics package that describes the physical and chemical properties of the chosen chemicals – Steam Tables.
- Select the unit operations (a simple Heater)
- Define all required inputs and the heat duty of the heater.
- Run the program and examine the results

Procedure to Create a Simple Heater Model:

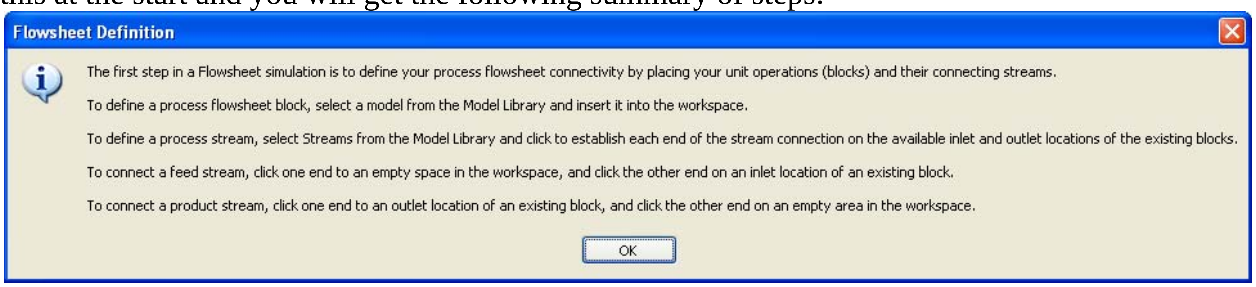
1. Start Aspen Plus User Interface by going through the start menu, Chemical Engineering, AspenTech, Aspen Engineering Suite, Aspen Plus 2006, Aspen Plus User Interface



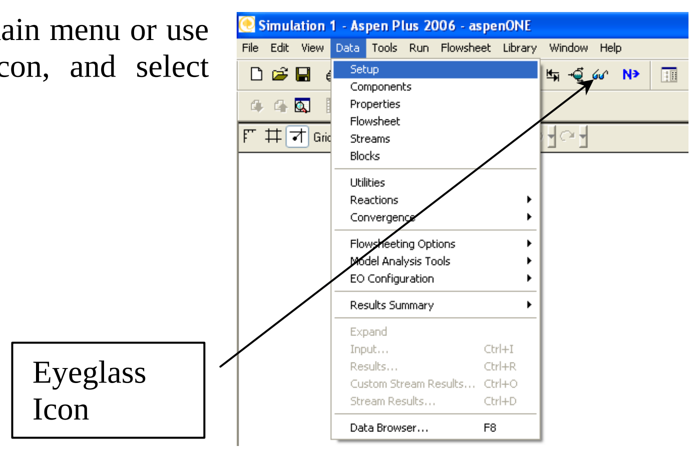
2. Create a new simulation using a blank simulation and server type Local PC

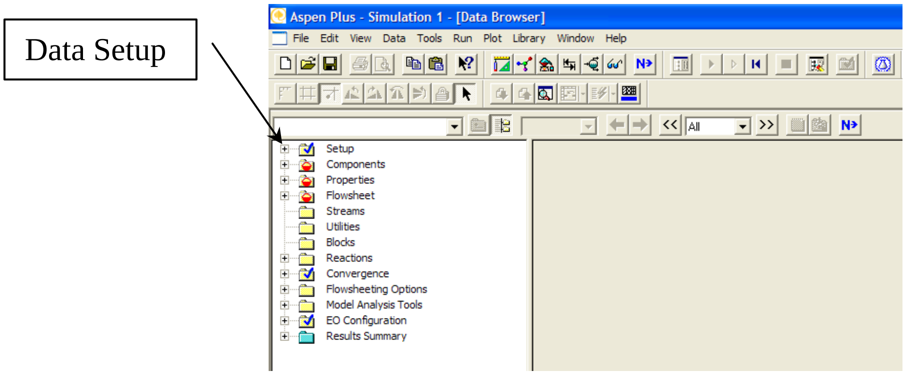


3. One way to proceed through the setup screens is to click  to take you to next action. Do this at the start and you will get the following summary of steps:

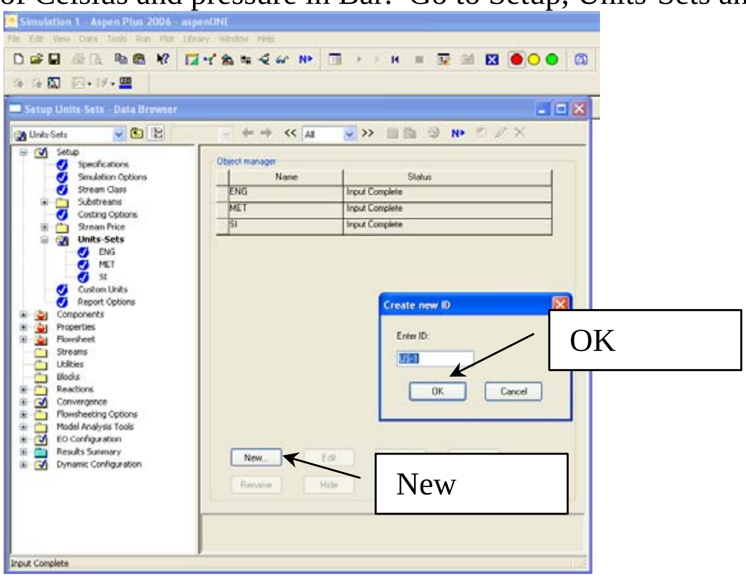


4. Choose *Data*, *Setup* from the main menu or use *Data Browser* from the eyeglass icon, and select Setup.

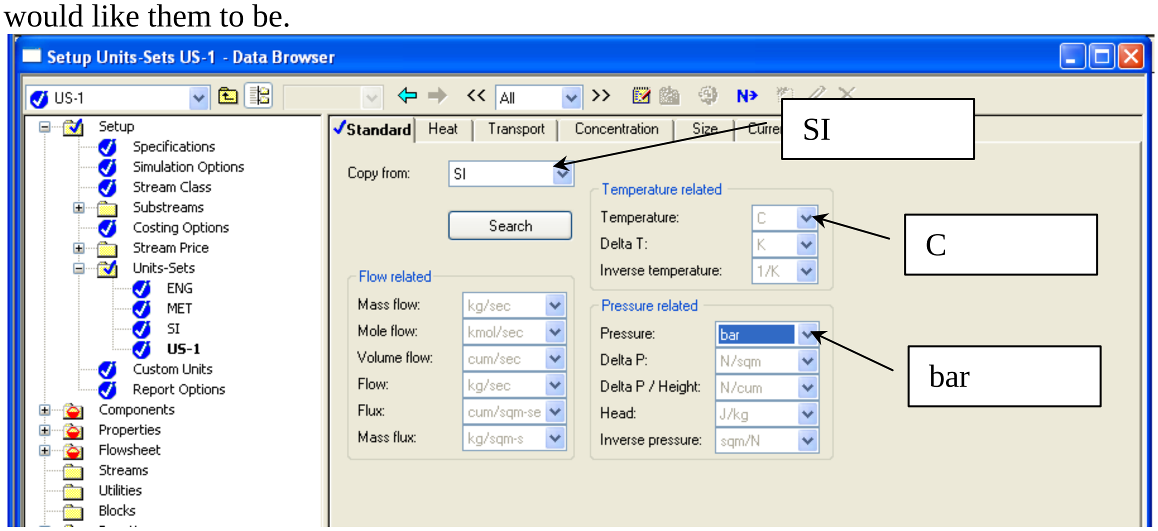




5. We will now define a unique unit set that is in the metric system with units of Temperature of Celsius and pressure in Bar. Go to Setup, Units-Sets and then press the New… button.

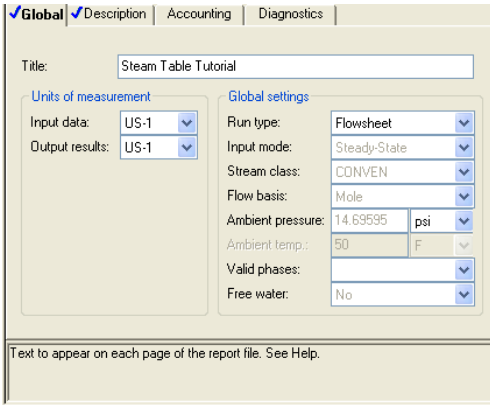


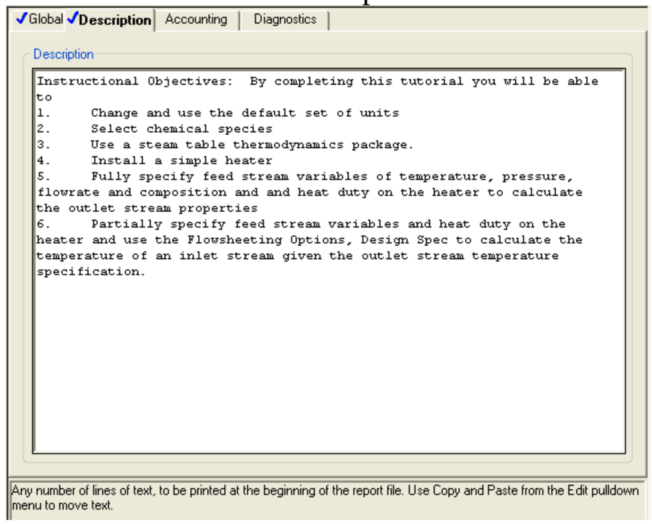
6. Choose SI and C for Celsius. You can always go back and adjust the units to what you would like them to be.



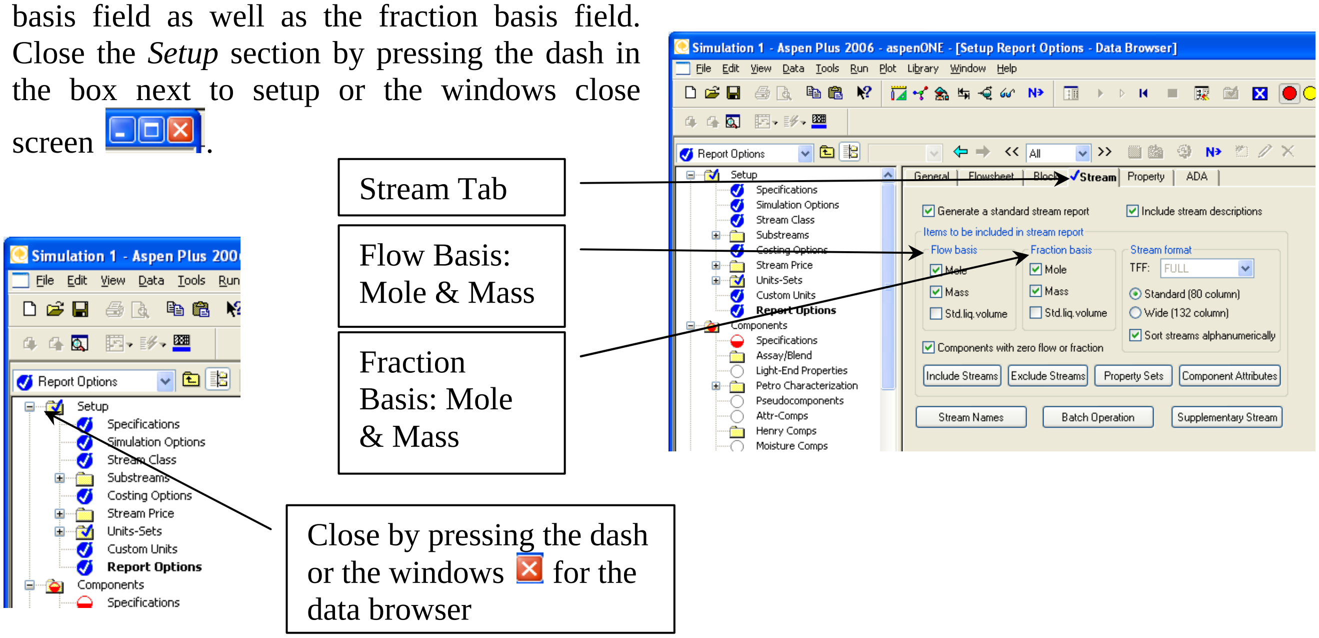
7. Next choose bar for Pressure. You can always go back and adjust the units to what you would like them to be.

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



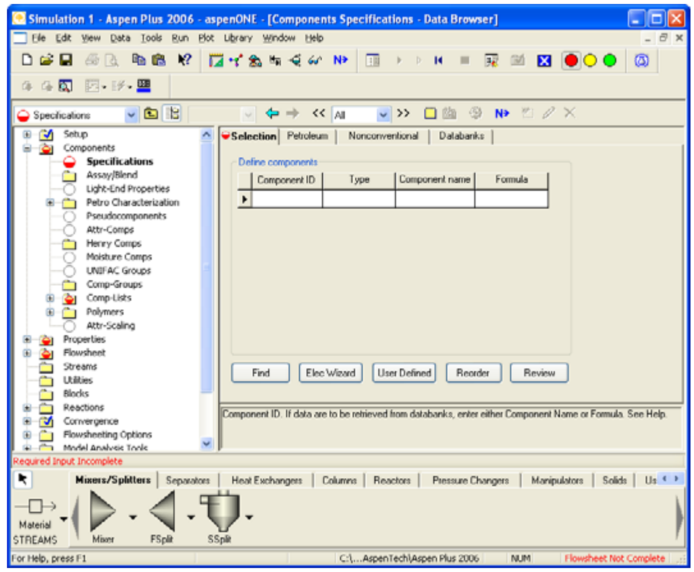


9. Before proceeding, move to *Report Options* where you can specify the information that will be printed in a final report. Under the *Stream* tab, select both mole and mass in the flow basis field as well as the fraction basis field. Close the *Setup* section by pressing the dash in the box next to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

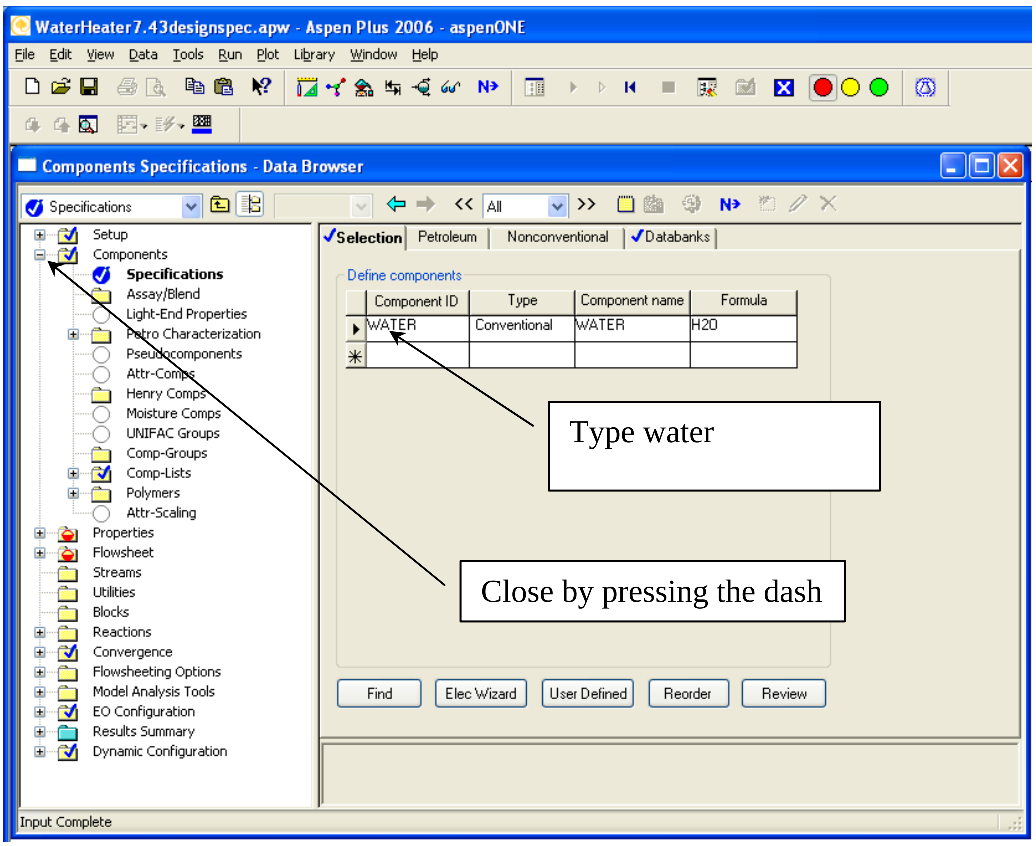


10. Click to take you to next Input step. Using the Next button will help guide you to each step that needs to be performed.

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



12. Next select the chemicals for your reaction system. For this simulation just type water and press enter.



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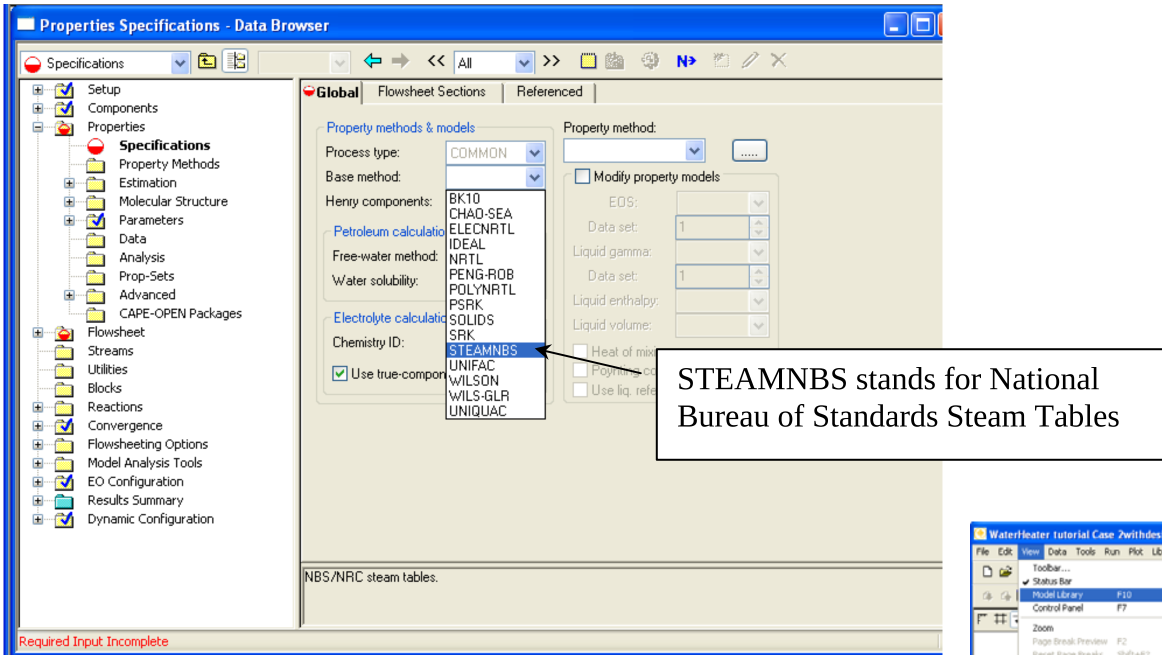
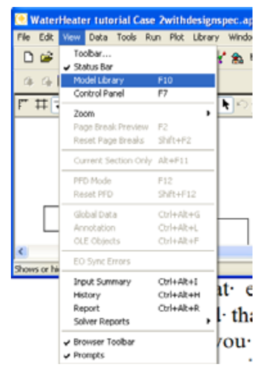
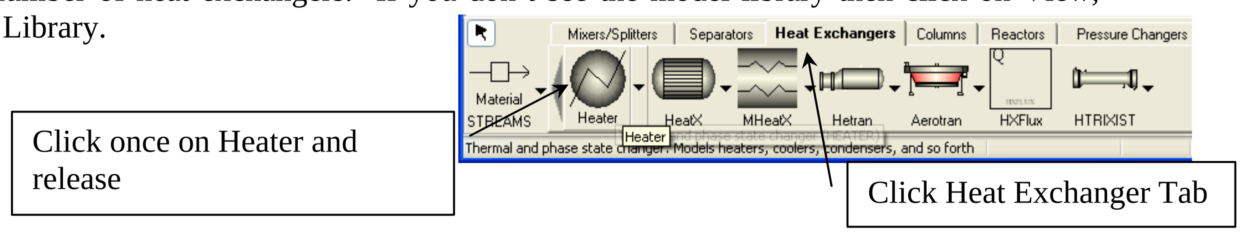
13. Next, select as base method for system properties, by selecting *Properties*, *Specifications*. Since is water you will use the steam tables. Choose STEAMNBS under the *Base method* tab. This is an equation of state that was developed for water. The other option is the ASME steam table correlations. Close the *Properties* section and the *Data Browser* (and all other windows) revealing the blank Process Flow Window.

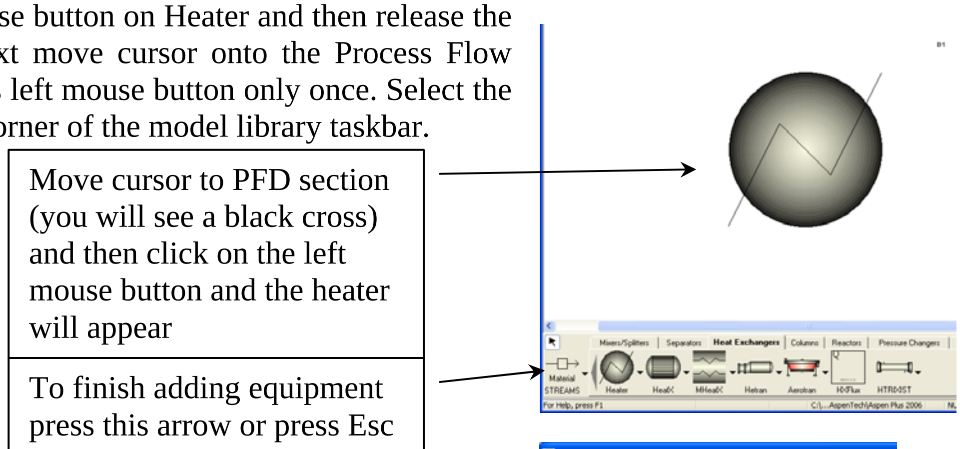




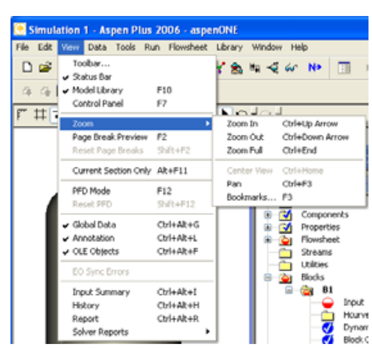
14. You are now ready to setup your flowsheet. Close the data browser menu screen by clicking on the ☒. You should see the blank Process Flow Window. You will now create a simple heater simulation. Note there are many very complicated types of heat exchangers in this menu and it is not recommended that you use other models until you learn more about this type of equipment. Click on the Heat Exchangers tab and you will see a number of heat exchangers. If you don't see the model library then click on View, Model Library.



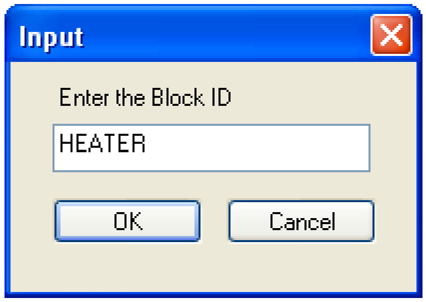
15. Click with the left mouse button on Heater and then release the left mouse button. Next move cursor onto the Process Flow Window and then press left mouse button only once. Select the arrow in the very left corner of the model library taskbar.



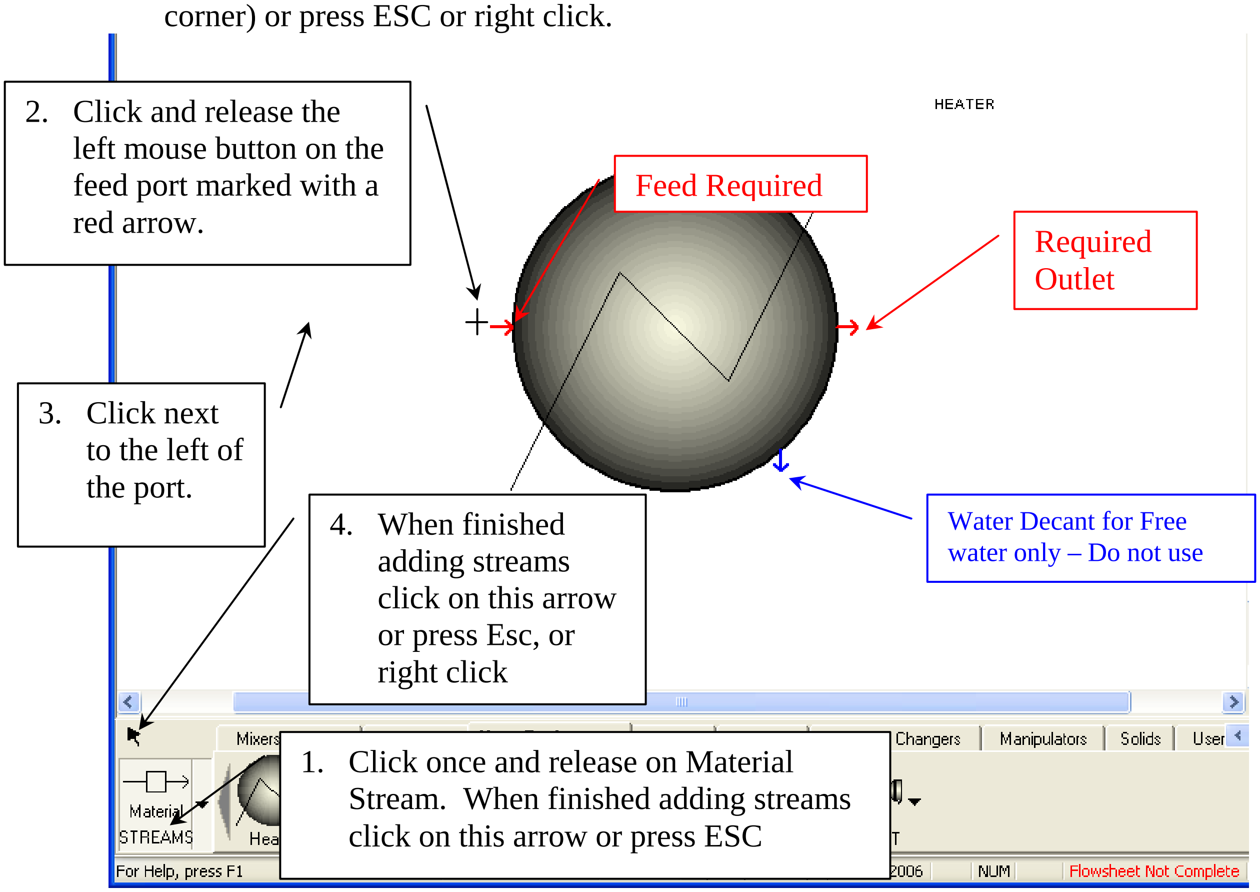
16. To see a larger image go to the view menu and adjust the size. Zoom Full (Ctrl+End) will zoom and center the object. Pan performs a similar function.



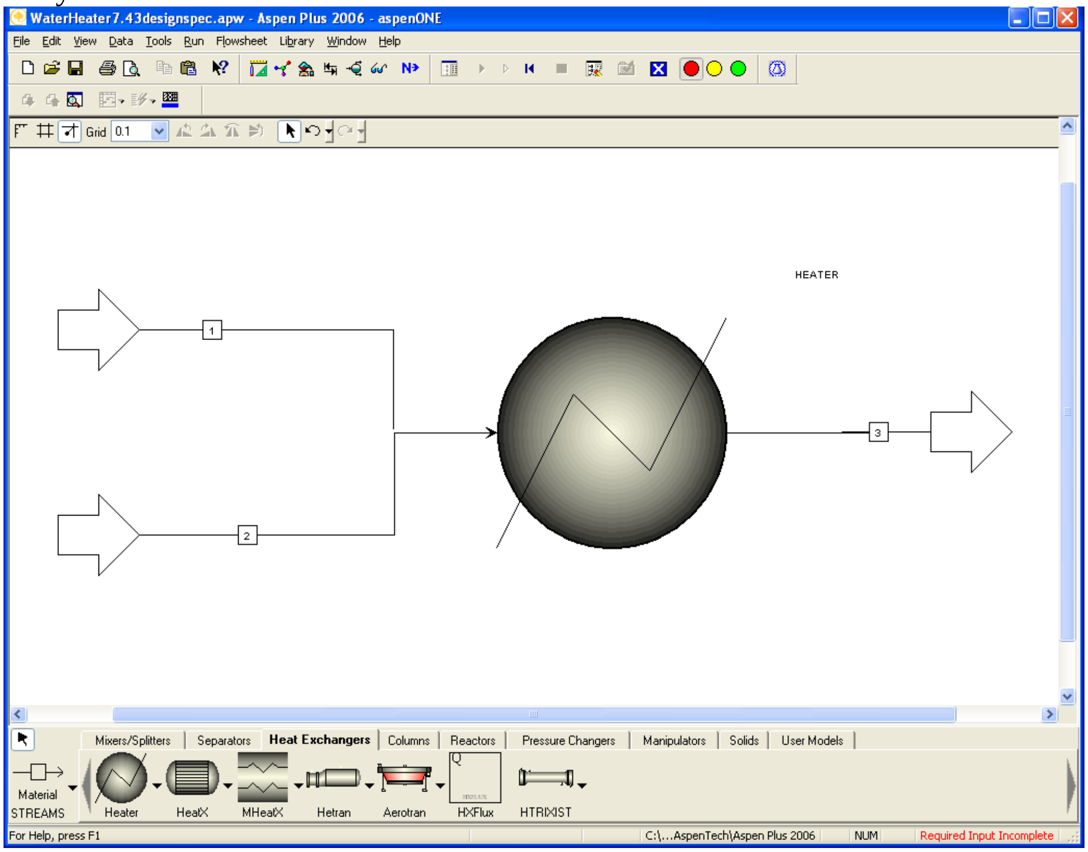
17. Rename the separator using a descriptive name by right clicking and selecting *Rename Block.*



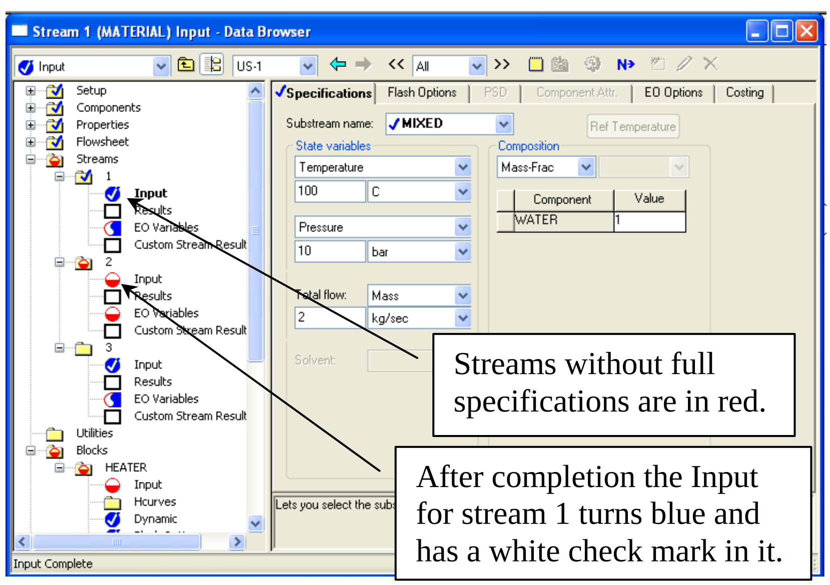
18. To add feed and effluent streams, use the *Model Library* to select the *Material STREAMS* tab in the lower left-hand corner and click once. This will allow you to place multiple streams as needed. Move the cursor, now a crosshair, onto the process flowsheet. Notice that ports on the flash drum are 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.
19. Click once on the feed port and release. Then click to the left of the heater. You will have added the feed stream 1. Repeat to add Feed Stream 2.
20. Now add the outlet stream by clicking on the outlet and releasing. Next click to the right of the heater and release. Press the black arrow next to the material stream block (bottom left corner) or press ESC or right click.



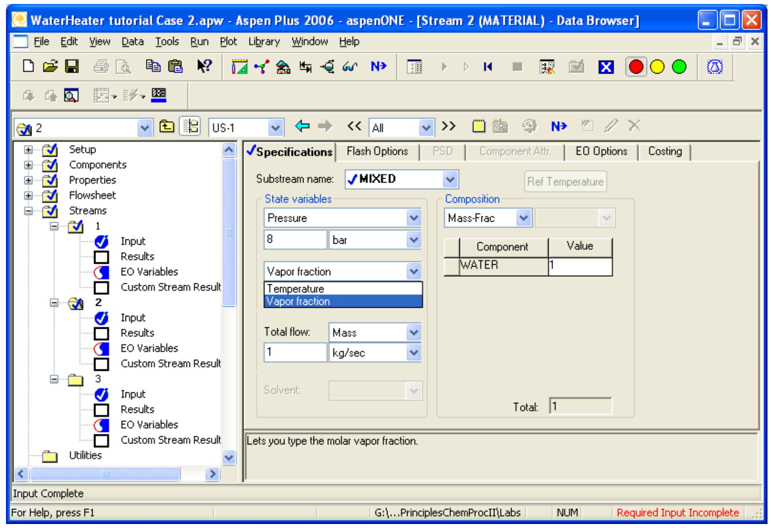
21. You will need to modify the streams by dragging the lines so that they look like the figure below. If the streams did not attach then, right click on the stream in question and select *Reconnect Source* or *Reconnect Destination.* Rename streams by right clicking on them so that you have a the feed streams labeled 1 and 2 and the outlet 3.



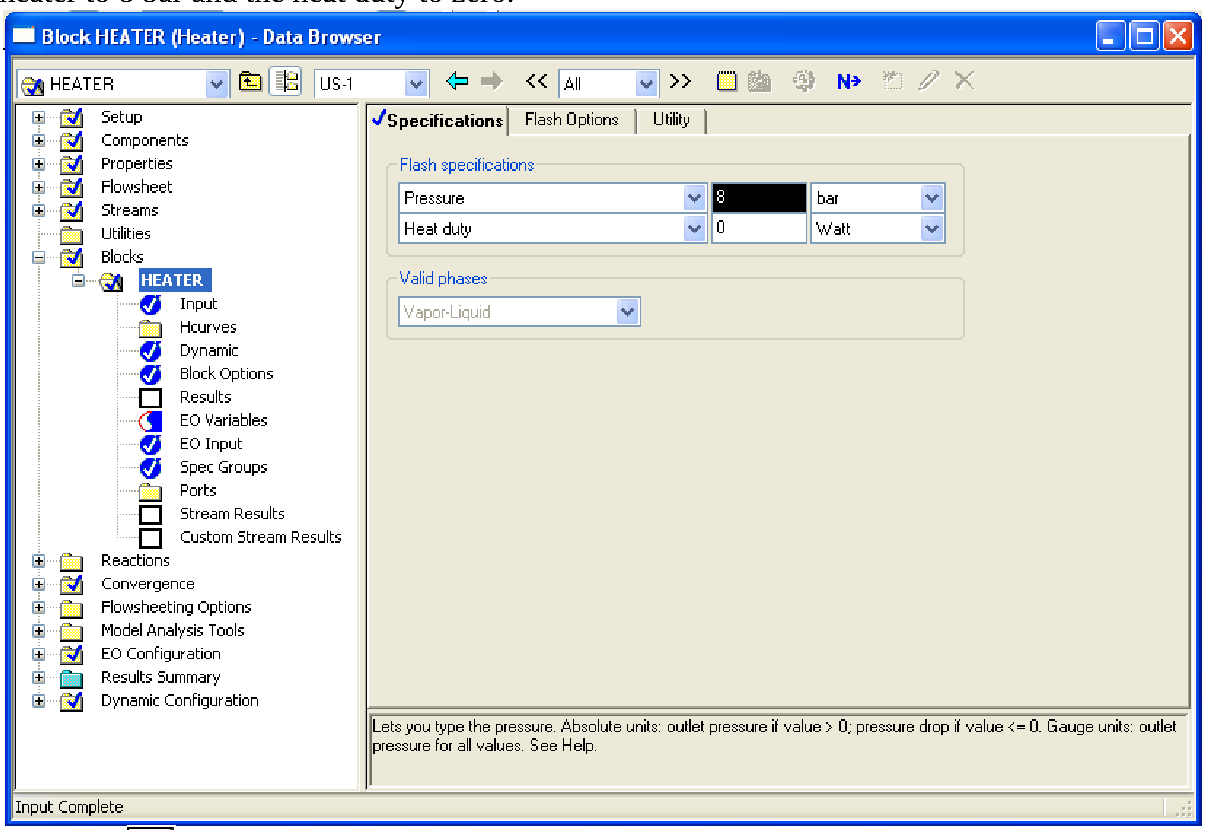
22. Specify the conditions of the feed stream 1 (Double click on the stream or right click on it and then choose input). The inlet pressure is P= 10 bar, T=100°C, the total mass flowrate is 2 kg/s and the mass fraction of water is 1. Yes it is silly to need to type this in but the program needs this specification. Another way to do this is to specify a mass flow in the composition and leave the Total flow blank. Notice that the Input is completed as marked by a blue circle with a white check mark in it. Stream 2, the second inlet stream needs to be specified next and it is still red.



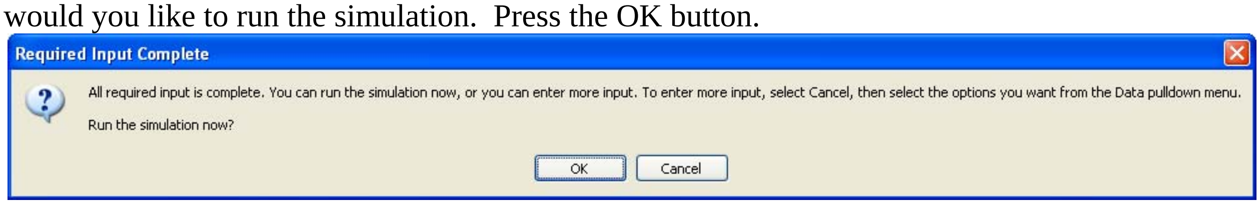
23. Specify the conditions of the feed stream 2 (Double click on the stream or right click on it and then choose input). The inlet pressure is P = 8 bar, and the stream is a saturated vapor. The total mass flowrate is 1 kg/s and the mass fraction of water is 1. What value must the vapor fraction be to specify a saturated water vapor at its dewpoint (saturated steam as opposed to saturated liquid water)? Notice that the Input is completed as marked by a blue circle with a white check mark in it.

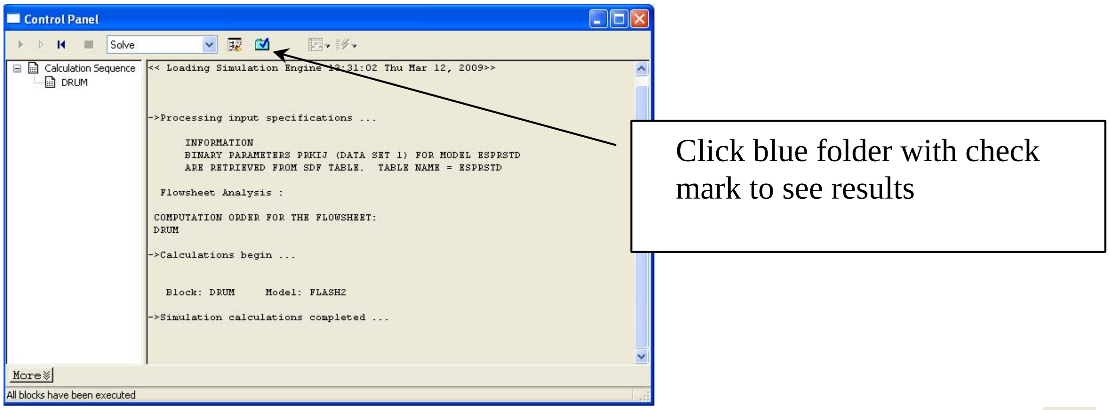


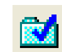
24. Now specify the heat duty and the pressure in the heat exchanger. Set the pressure of the heater to 8 bar and the heat duty to zero.

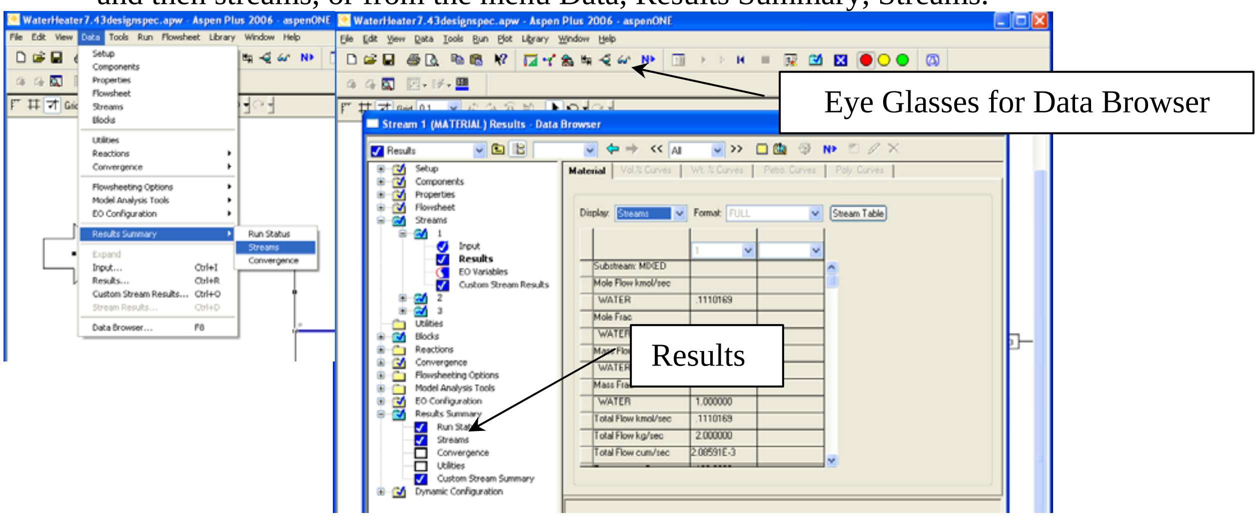


25. Press the  button and it should give you a pop up screen that everything is complete and would you like to run the simulation. Press the OK button.





26. Now you need to look at the results. Click on the blue folder with a check mark  on it to see the results. Other options are to click on the eye glasses and choose Results Summary and then streams, or from the menu Data, Results Summary, Streams.

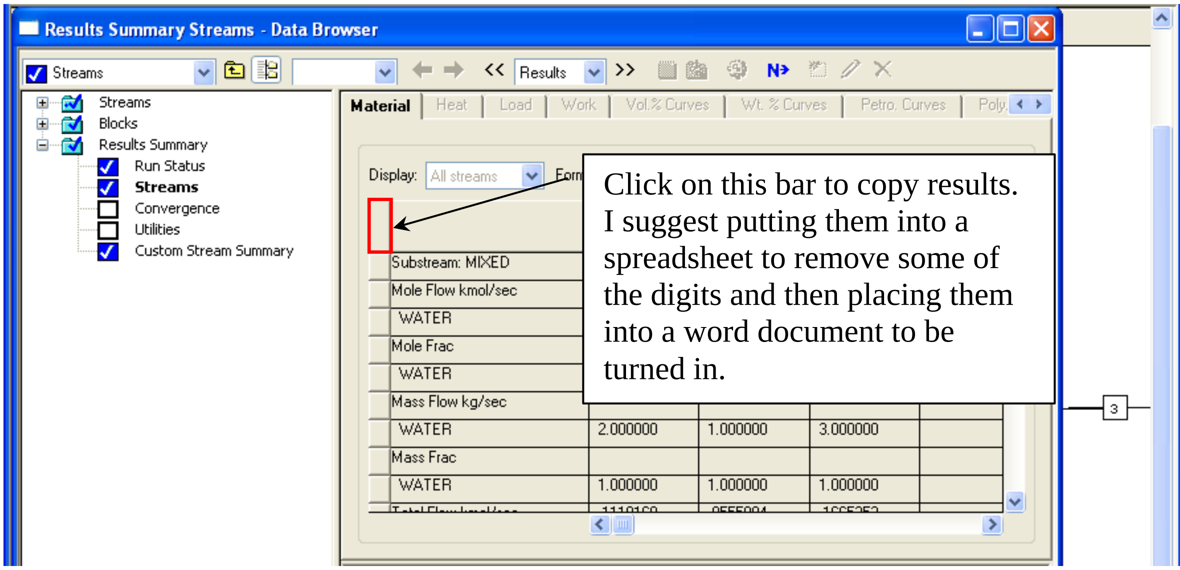


27. Save the file on your galaxy drive. File, Save as, and change the path to your personal galaxy drive. I would suggest always saving your files with a unique descriptor (your name). The files are always printed with your filename showing on the page.

28. Compare your hand calculations with the results. Fill out the following table. (See next step for a method to cut and paste from ASPEN).

Table 1: Case 1 a "Adiabatic Heater" with Feed Fully Specified

Stream Name	1	2	3
ASPEN Temperature (°C)			
Hand Calculation Temperature (°C)			
ASPEN Vapor Fraction			
Hand Calculation Vapor Fraction			
ASPEN Enthalpy (kJ/kg)			
Hand Calculation Enthalpy (kJ/kg)			



29. Compare your numbers and make a comment on the reference state used by ASPEN for the steam tables in the STEAMNBS package. Explain the differences between values of enthalpies. What is the reference state for the NBS table? To determine the reference state compare the heat of formation value of liquid water at 25°C and 1atm given in your textbook with the enthalpy value of a stream of liquid water at the same conditions. (e.g. do another run on ASPEN)

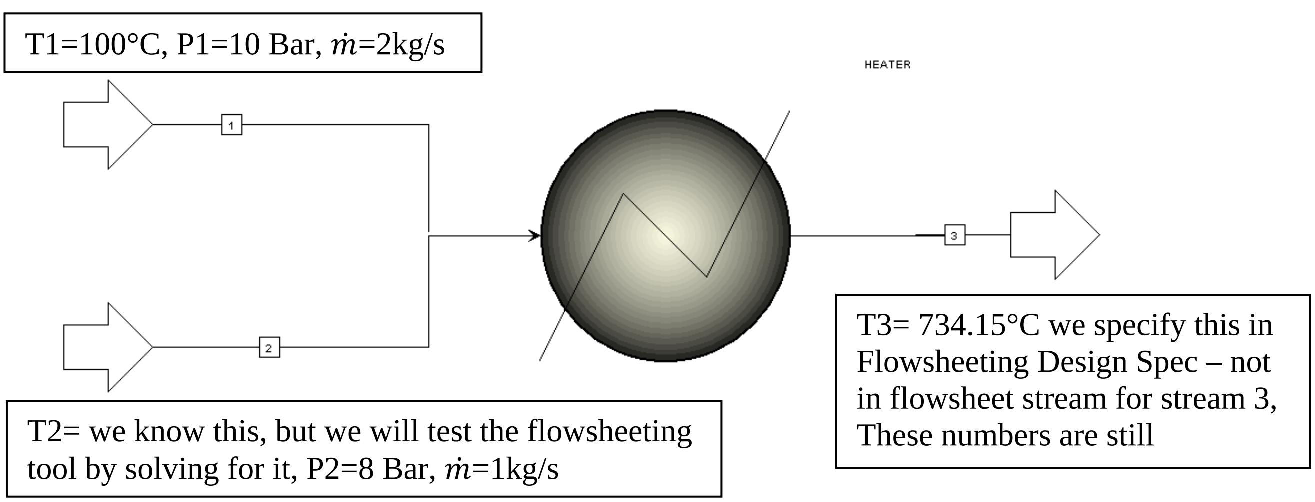
CASE 1b:

30. Run Case 1b by adding a heat duty of 8400 kJ/s to the heater. Compare your ASPEN outlet stream temperature to the temperature calculated by hand. Comment on the difference between these answers.

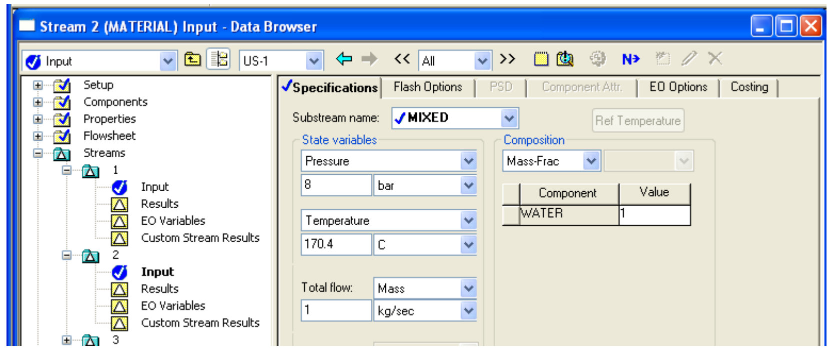
CASE 2: Using Flowsheeting, Design Spec to solve for an inlet condition

The overall process for the third simulation will start by first getting the Flowsheeting Design Specification tool to work on the case you have just completed (Case 1b). Then you will modify your stream conditions to those of Case 2.

The following is the current Case 1b:

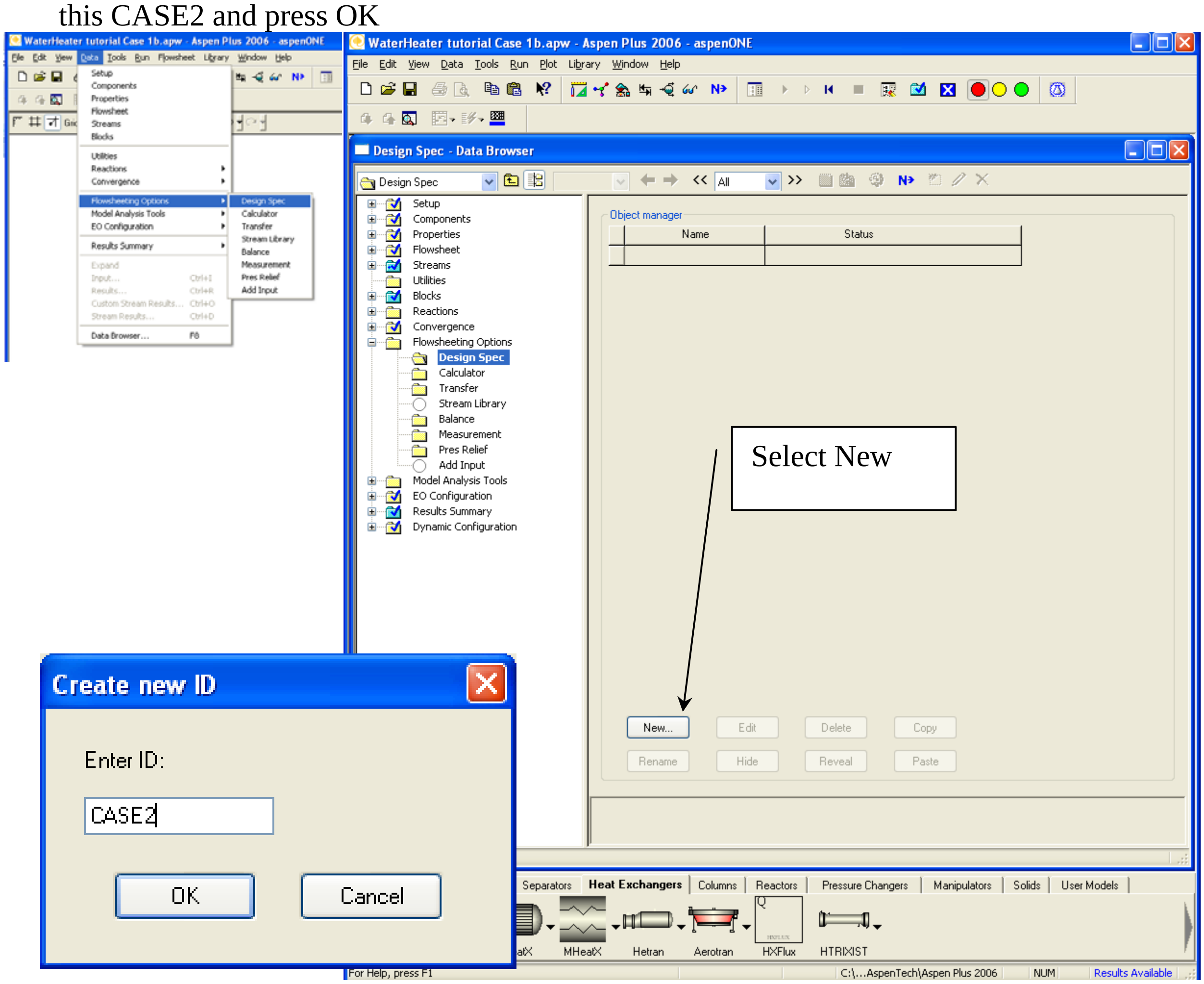


31. For this practice simulation we will repeat case 1b. You will specify the outlet temperature to that obtained in the last simulation. Since we didn't specify the temperature initially, you should change the inlet specification from vapor fraction to temperature. Check to see that a temperature specification of 170.4°C will give the same answer as the previous solution. Comment on the outlet temperature that was obtained. Why was this temperature lower than the previous specification? Look at all the conditions of stream 2 and compare it to the specification of pressure and vapor fraction.

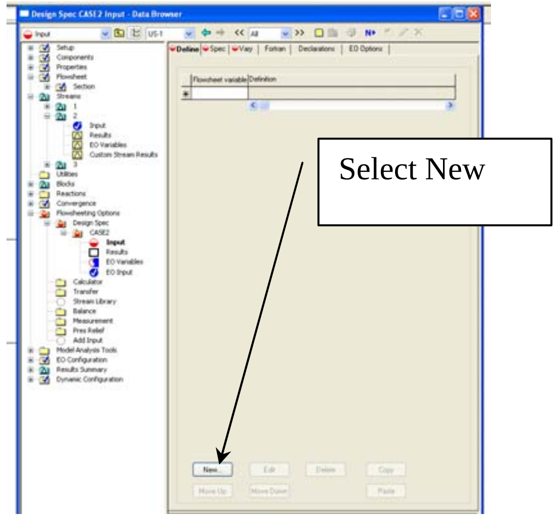


32. The Flowsheeting Options, Design Spec is a tool that will use a root finding method such as Secant, Wegstein, or Newton (See Felder & Rousseau[1] Appendix A.2). You can approximate this by guessing an inlet temperature of stream 2 and calculating an outlet temperature. Try values of 150°C and 200°C.

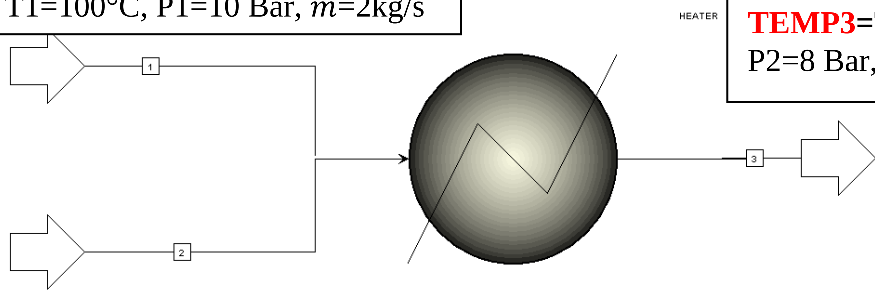
33. Go to Data, Flowsheeting Options, Design Spec. Next press the New… button and rename this CASE2 and press OK



34. Press the New Button.



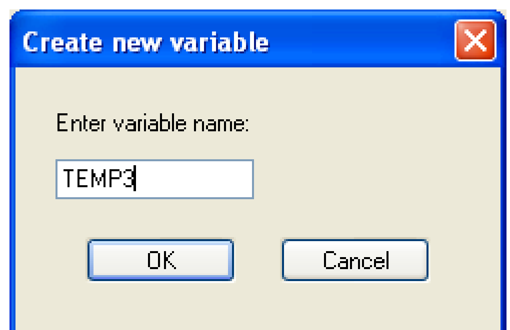
T1=100°C, P1=10 Bar, $\dot{m}$=2kg/s

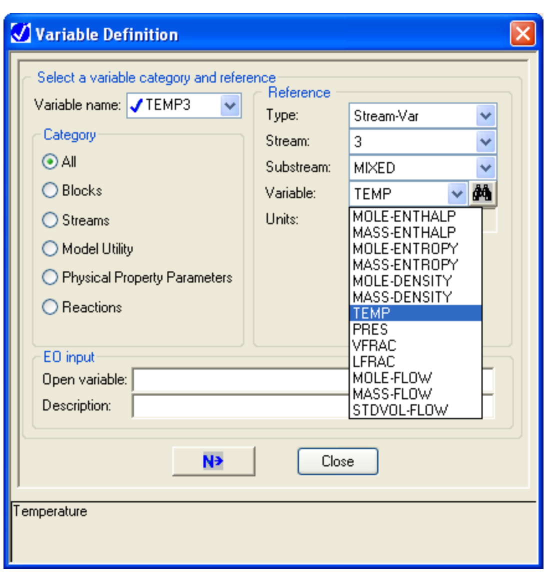


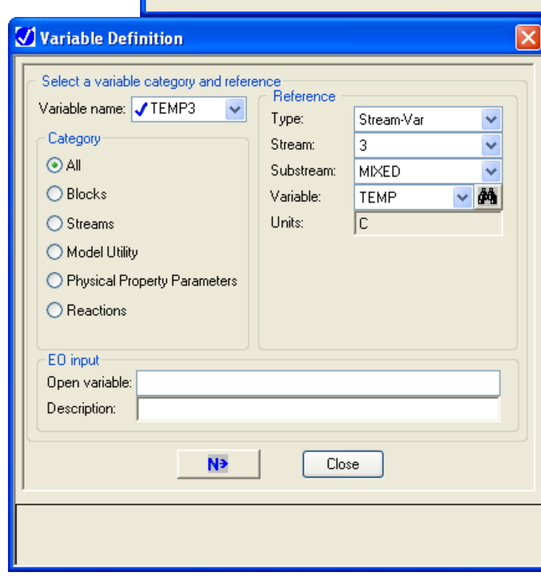
Iterate on T2 to find **TEMP3=T3** = 734.15°C, P2=8 Bar, $\dot{m}$=3kg/s

T2= **first guess that will be varied**, P2=8 Bar, $\dot{m}$=1kg/s

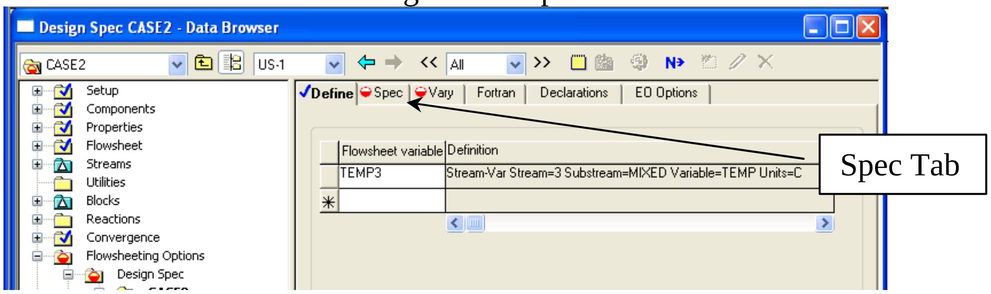
36. Give the variable a name TEMP3 which will be the specified variable.
37. Then specify Type – stream variable from stream 3 and the variable is temperature.



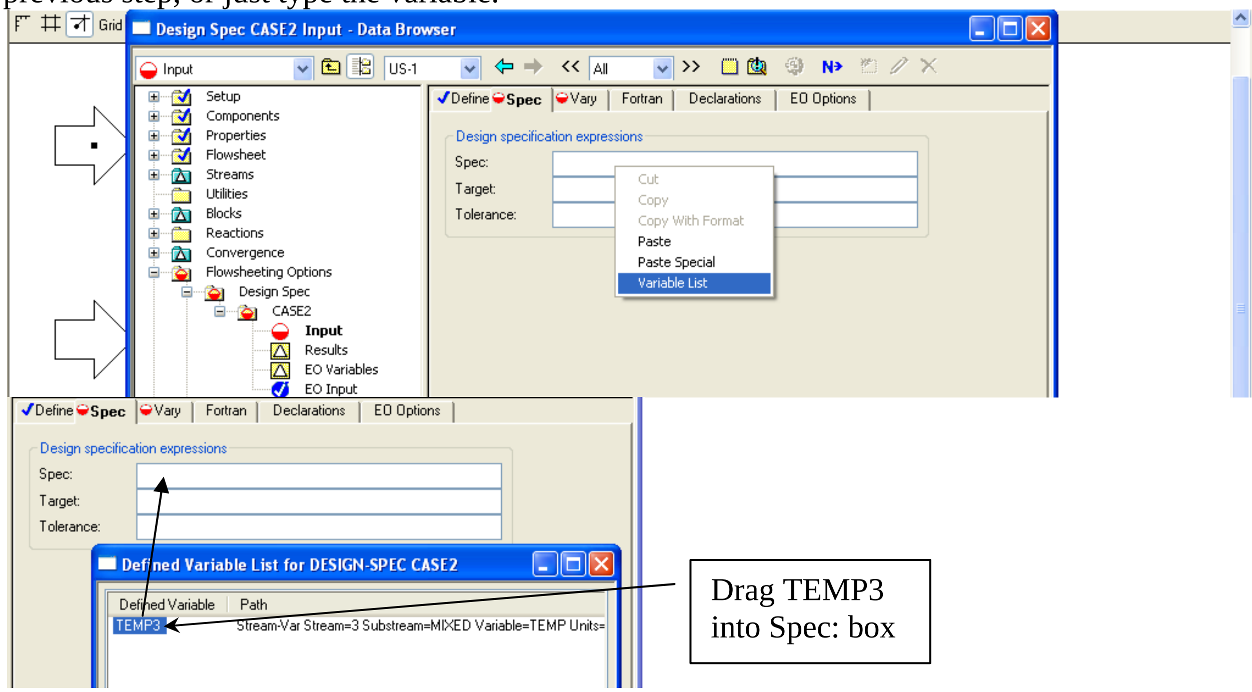




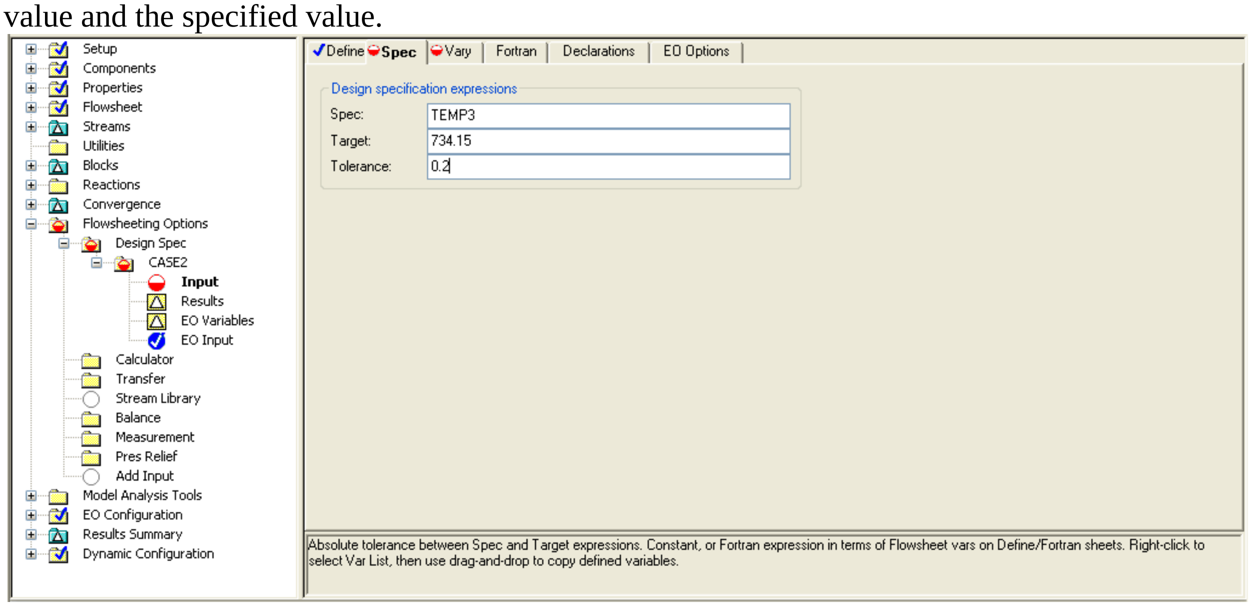
38. Press the close button and then go to the Spec tab



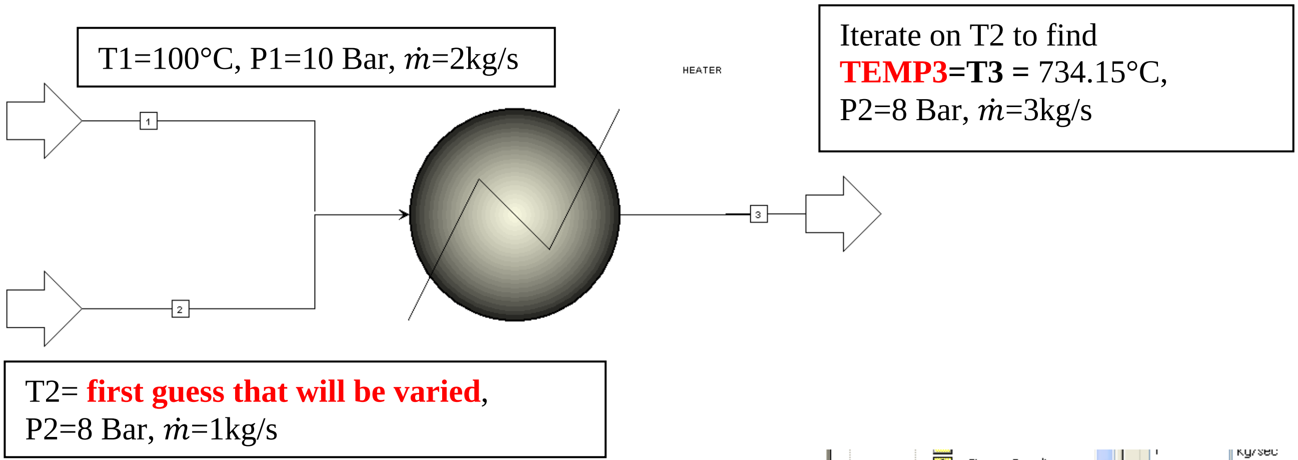
39. In the Spec sheet right click in the Spec: box to drag in the exact variable defined in the previous step, or just type the variable.



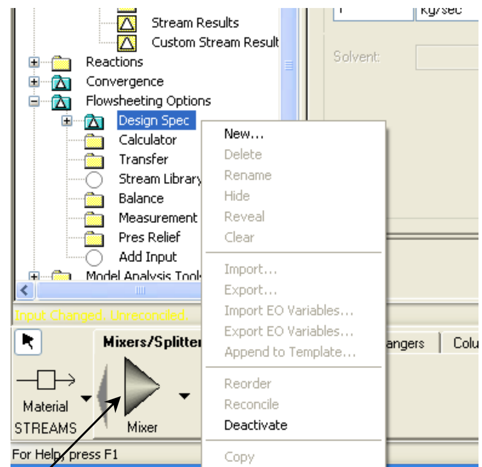
40. Then fill in the numerical value for the specification and a Tolerance between the calculated value and the specified value.



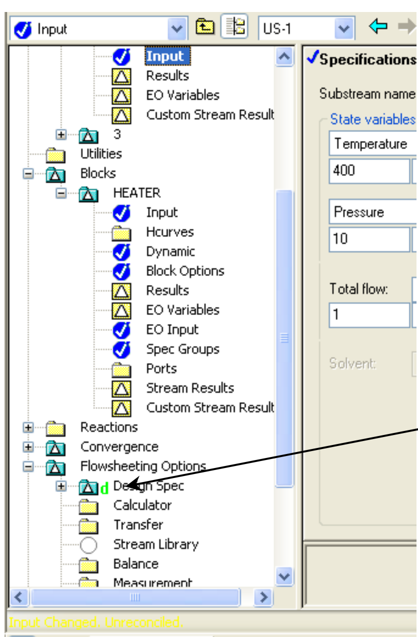
41. Select the Vary Tab and specify that you want the program to vary the temperature in stream 2 until the temperature in stream 3 is equal to 734.15°C±0.2°C.



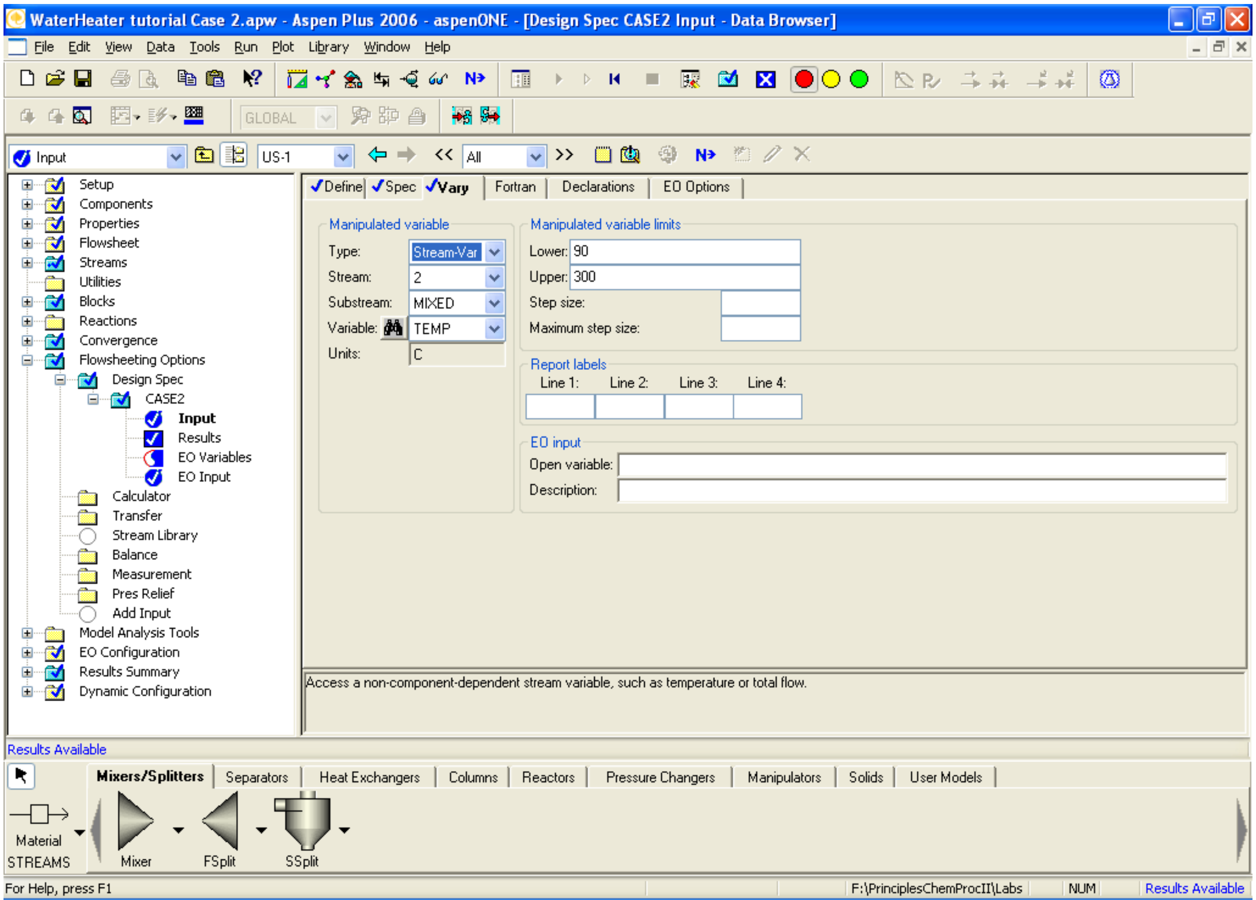
42. To find lower and upper limit values a few trials could be conducted to make sure that you are in range. To do this you must first turn off the flowsheeting specification. Go to Flowsheeting Options and right click on Design Spec. Choose deactivate and this will deactivate the Flowsheeting tool. Perform several trials by manually varying the temperature in stream 2 to find an upper and lower bound. Then place a new initial guess in the stream 2 temperature space and then reactivate Design Spec and type in appropriate bounds on the temperature 2 for this new problems



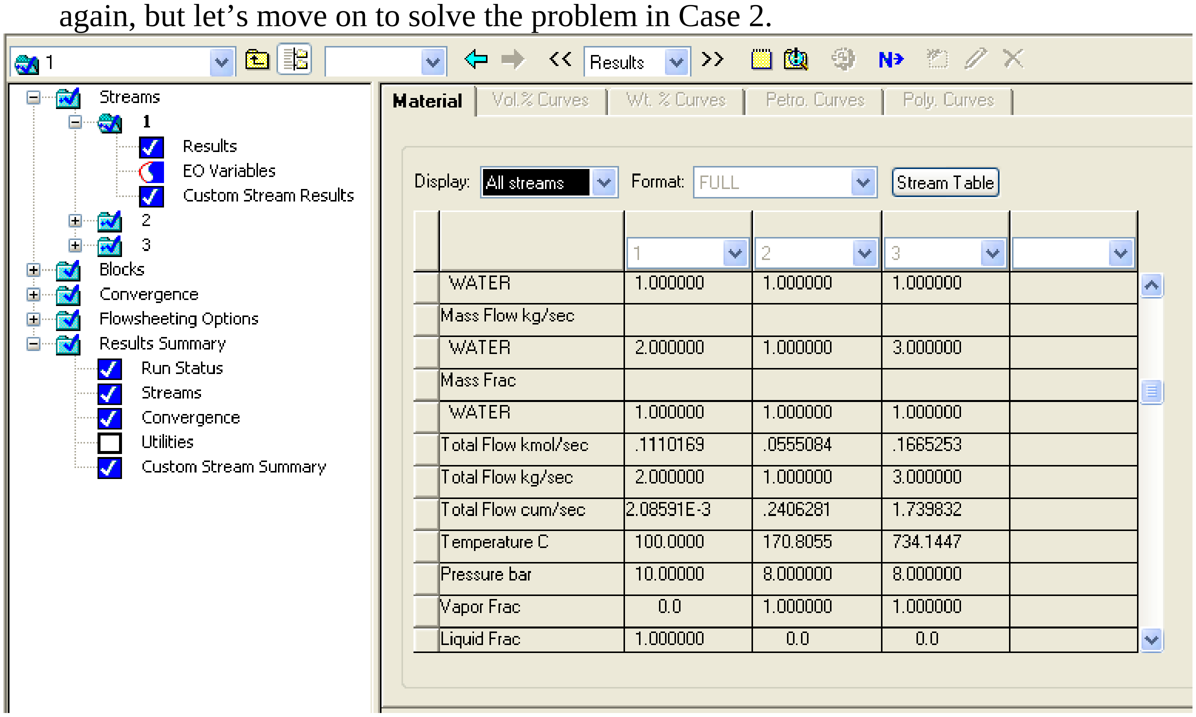
Right click on Design Spec



Choose Deactivate and a green d appears.



43. Now we are ready to solve. Press the next button and run the solver. You should now have the solution that you found for Case 1b in which the temperature of stream 3 is 734.14°C and the temperature of stream 2 is 170.4°C. To improve the accuracy you could run this again, but let's move on to solve the problem in Case 2.



44. CASE 2: For this problem we will go back to our heater in case 1b. For this simulation you have been requested to achieve a temperature in stream 3 of 700°C at 8 bar using a lower heat duty on the heat exchanger of 7236 kJ/s. You have the same feed stream 1 at 100°C and 10 Bar and a mass flowrate of 2 kg/s. For this problem you must determine the temperature of the second feed stream which will be at a new pressure of 10 Bar and mass flow rate of 1 kg/s. Determine the inlet stream temperature of stream 2. To run this simulation change the values of stream 2 and change the specification of TEMP3.

45. 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 from the case 2 simulation:
  - filename.apw (the case file for running Aspen)
  - and the report file filename.rep. This file should contain the case for your hand calculation.

  Word document containing answers to the questions
  1. Summary table of Case 1a (See page 11)
  2. Comparison of values for Case 1a between hand calculation and ASPEN. (See page 12 number 29)
  3. For Case 1b, compare your ASPEN outlet stream temperature to the temperature calculated by hand. Comment on the difference between these answers.
  4. Comparison of using a temperature specification of 170.4°C for case 1b compared to specifying the vapor fraction. Explain findings. (see page 13 Number 0).
- **Submit the hand calculations as instructed**
  - **Case 1a&b**
  - **Case 2**