

# Introduction to HYSYS 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 Hyprotech Inc. This program is used by industry to design and simulate process plants such as oil and gas refineries, chemical and pharmaceuticals production facilities. A typical sampling of well-known companies using this software are given below:

- DuPont, Eastman Kodak, Monsanto, Hoechst Celanese, Rohm & Haas
- Shell, Amoco, Exxon Chemical, Olin, Conoco, Phillips
- Foster Wheeler, Arthur D. Little, Ballard, Koch
- Hoffman LaRoche, International Flavors and Fragrances,

This software is written in C++ which is a language that you have learned. The cost of this software is approximately \$45,000 for the dynamic version and \$20,000 for the steady-state version. This price is for only one user! For more information on Hyprotech go to [www.hyprotech.com](http://www.hyprotech.com)

The overall process for this simulation is to

- Select a thermodynamics package that describes the physical and chemical properties of the chosen chemicals
- Select the unit operations
- Define all required inputs and output streams. Specify required values of temperature, pressure, flowrate and chemical concentration.

### Start your computer:

Rowan University has a license to run HYSYS PLANT version 2.4, which is both a steady state and dynamic simulation program.

For convenience Hyprotech suggests that you copy the HYSYS directories to your personal drive on galaxy. These are located in [\\galaxy\\public\\chemical\\engineering\\HYSYS](http://\\galaxy\\public\\chemical\\engineering\\HYSYS) (To do this you may need to map a drive (Start, Windows Explorer, Tools, Map Network Drive....) In these directories you will save your configuration files and cases.

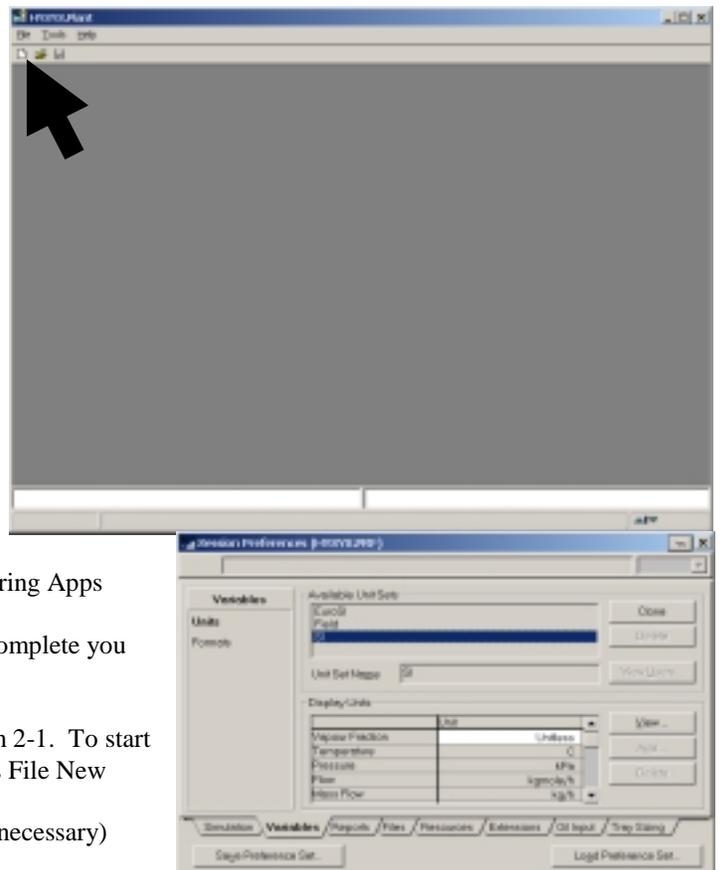
In HYSYS there is a limited online **Help** package, which can be obtained using the Help command from the menu bar or by pressing the F1 key. There is an extensive collection of manuals that can be accessed from [\\engnet1\\apps\\Hysys\\_Doc\\Menu.pdf](http://\\engnet1\\apps\\Hysys_Doc\\Menu.pdf). Remember that we are running HYSYS PLANT.

- 1) Start HYSYS PLANT  
**Third Floor Lab** (windows NT) Start => Engineering  
Network apps => Engineering Apps => HYSYS Plant  
**First floor labs** (windows 2000) Press Start => Engineering Apps  
=>HYSYS Plant

This package will take about a minute to start up and when complete you will see the screen given above.

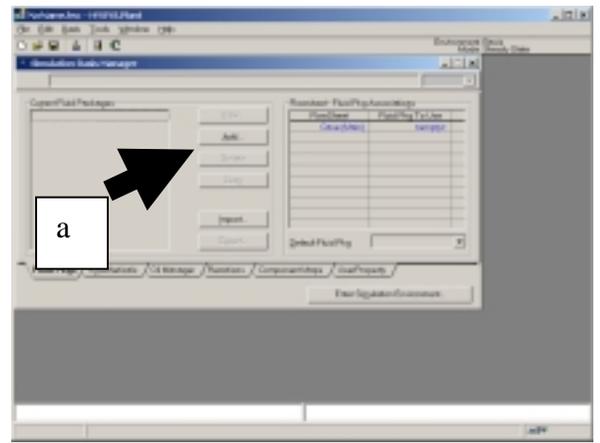
In this exercise we will complete Wankat's Example Problem 2-1. To start a new case click on the white page icon or use the commands File New Case. See previous page.

- 2) Change your units from American engineering to SI: (if necessary)
  - a) Go to the command **T**ools, **p**references
  - b) Choose the Units tab



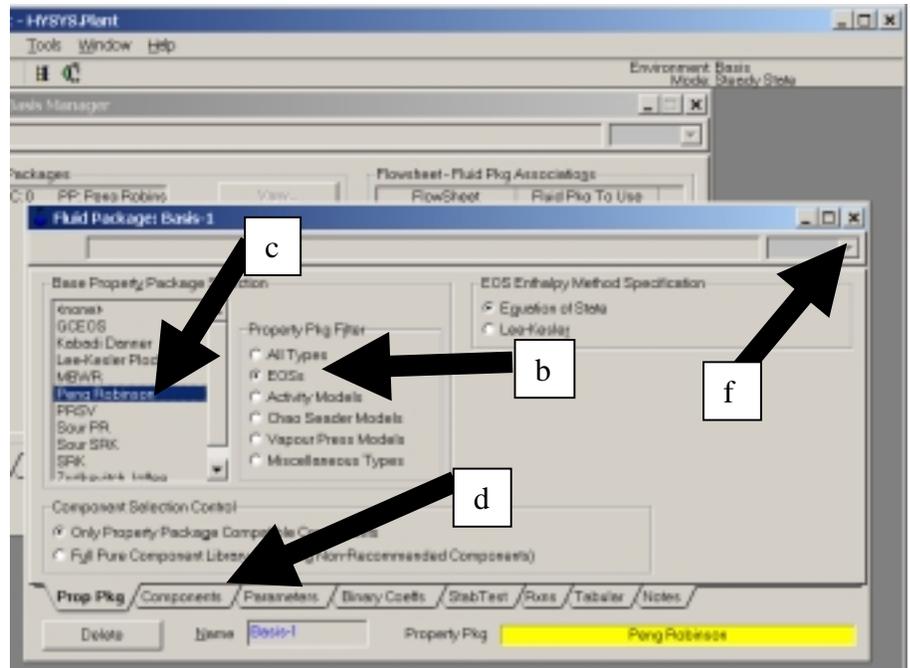
- c) Select SI
- d) Press Save Preference Set to your galaxy drive
- e) Press close.

The result will be the following menu screen to choose a thermodynamic property package. You will learn more about these packages in your chemical engineering thermodynamics course. We will use the Peng Robinson Equation of State (PR) our property package.

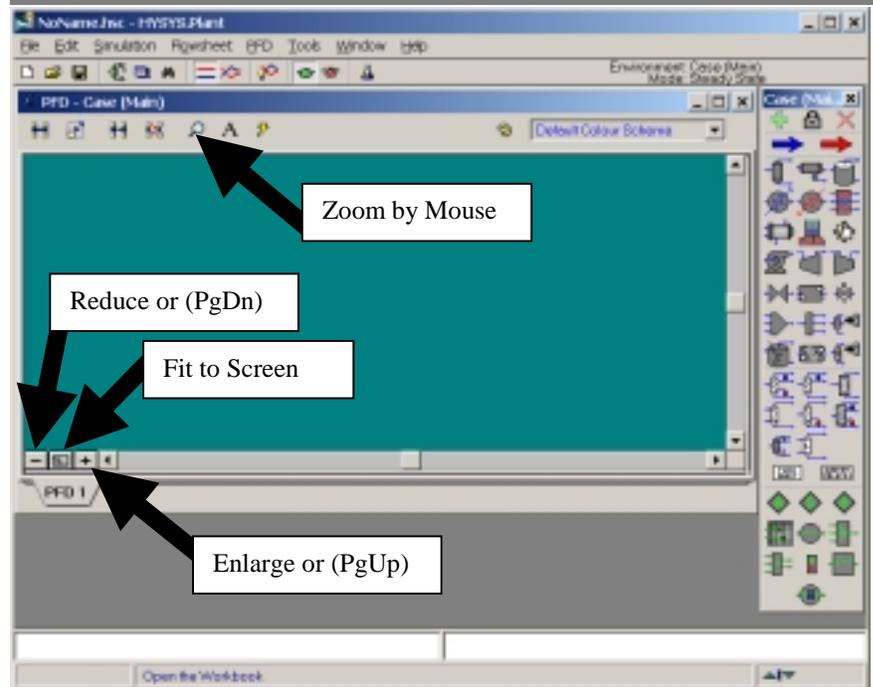


- 3) Choose the Property package and chemical components
  - a) Choose the button Add...
  - b) Choose EOS's
  - c) Choose PR
  - d) Press the Components tab
  - e) Add *i*-pentane, n-pentane, n-hexane by selecting each component and pressing the Add Pure button
  - f) Press the x or close button for **this screen**
  - g) Press the Enter Simulation Environment... Button (see figure above)

You should now see the following screen titled PFD - Case (Main). In the green screen you will construct a process flow diagram (PFD) of a flash process. The pictures of equipment shown to the right of the green screen contains the equipment that you will add. In this exercise we will add equipment simulating a flash.



- 4) 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. To determine which letter designates your galaxy drive, open Windows Explorer and find the letter corresponding to your "galaxy" drive.
- 5) Select a material stream by double clicking on the blue arrow and the menu labeled 1 will show on the pfd screen. Notice that a yellow warning sign appears telling you what is required: "Unknown Compositions." The other warning colors are red: "requires



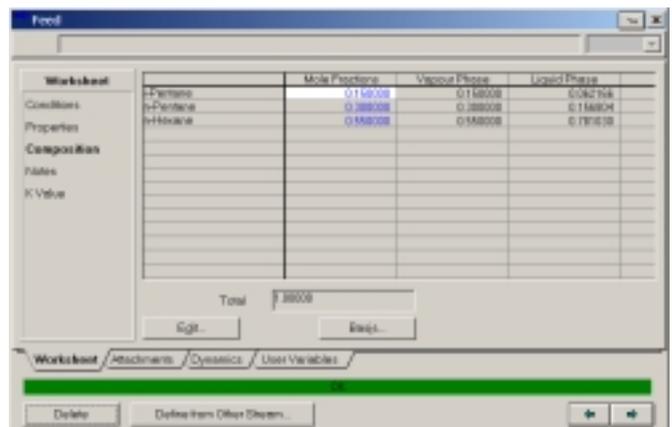
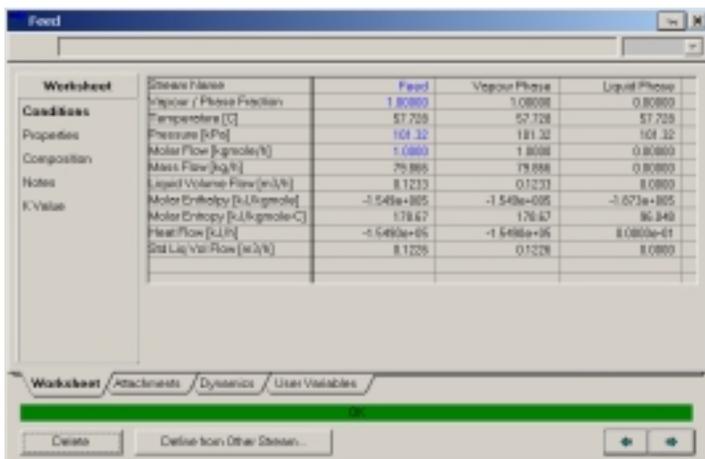
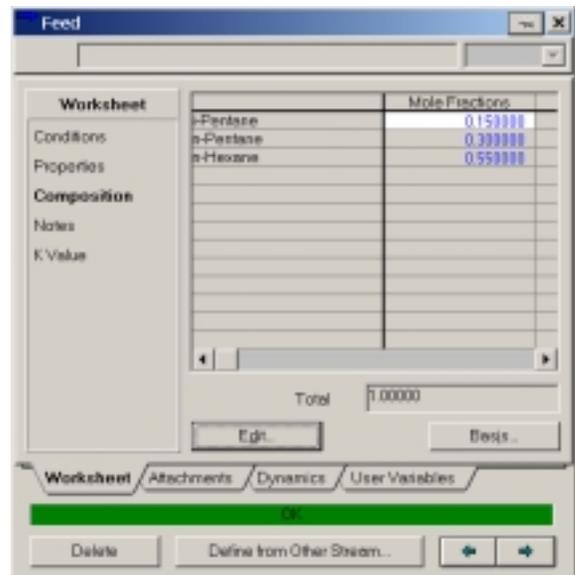
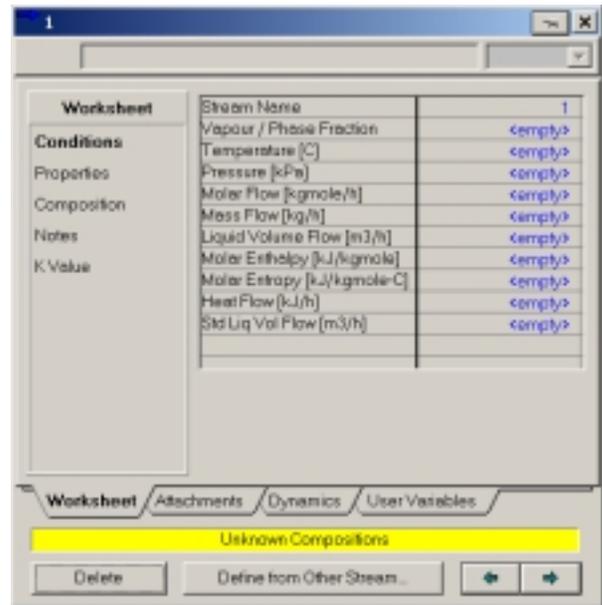
a feed stream,” and green for “OK” for it has been solved.

- 6) Fill out this menu as follows:
  - a) Stream Name: Feed
- 7) To enter your readings of temperature, pressure and flowrate for the Feed stream just type in the values given in the example problem 2-1. In this example you know the pressure and chemical compositions, and you will determine the bubble point temperature.
  - a) Type in your value of pressure as 1 atm. Type in the number, a space and the letters atm. Hit return and notice that it converts the units to SI automatically!
  - b) To specify mole fractions of each component do either:
    - i) select the composition options on the left side and click on the Edit button or
    - ii) double click on the cell next to Molar Flow [kgmol/h]:
  - c) Then type in the mole fractions of each component. See figure for values.
  - d) Check to see that you have 1.0 in the Total box, and then press the OK button.
  - e) Type any number in for the flow. I will use 1 kgmol/h.
- 8) To perform a dew point calculation type in a 1 in the Vapour/Phase fraction. To perform a bubble point calculation type in 0 in the Vapour/Phase fraction. Give the following: **Dewpoint temperature=** \_\_\_\_\_

**Bubble point temperature =** \_\_\_\_\_

You will notice after you enter the value of Vapour/Phase Fraction, the remaining values of this stream are calculated by HYSYS. The values in blue are the ones that you have entered and the values in black have been calculated by HYSYS. To enter in a new number you must first delete a stream value and type in a new number. Since most printers are use only black ink the values that you have specified are designated with an asterisk in the upper right hand corner.

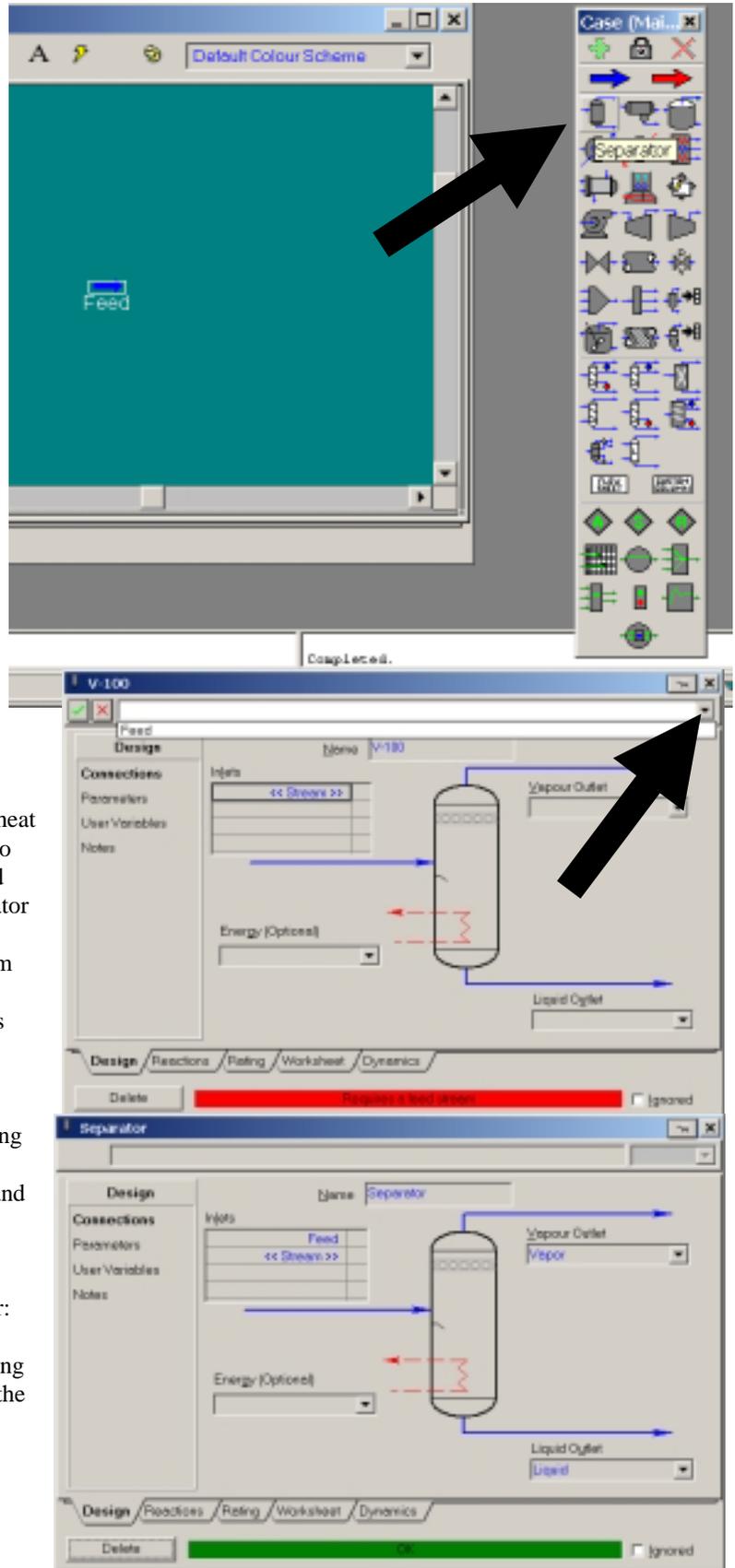
- 9) HYSYS also has the ability to show you the vapor and liquid phases of this stream. Move your mouse to the right edge of this window until you have a double arrowhead. Then click and drag to expand this window.
- 10) Save your case in your personal drive by executing the commands File, Save choose your drive letter and give a unique name to the case.



## Flash Calculations - Extension of Example 2-1

Flash calculations are performed for every stream in HYSYS. To perform a flash calculation on the stream labeled feed:

- 11) Delete the Vapor/Phase Fraction value. Type in a temperature value between the bubble point and dew point temperatures. ( $48^{\circ}\text{C} < T < 58^{\circ}\text{C}$ ). Your Vapor Fraction value should be between 0 and 1! You have just conducted an isothermal flash (all streams have the same temperature)! What are the mole fractions of the components in the vapor and liquid phases? Select composition and this screen will give the compositions of the vapor and liquid phases.
- 12) Now type in a temperature greater than  $60^{\circ}\text{C}$  or less than  $48^{\circ}\text{C}$ . Notice that the value of the vapor fraction is 1 and 0 respectively. A bubble point and a dewpoint calculation are only performed by specifying the vapor fraction as exactly 1 or zero.
- 13) In an isothermal flash you need to keep the temperature constant. This is easy to do in a chemical process simulator, but in the actual world you will need to either add or remove heat using a heat exchanger. Next you will need to separate these streams into a vapor and liquid stream. This can be done in a process simulator by installing a unit operation call a separator. This unit operation will automatically perform an energy balance to determine the energy required to perform an isothermal flash. This energy is called the heat duty.
- 14) Press F4 or select Flowsheet, Open Object Palette.
- 15) Select and add the separator by double clicking on the separator icon (If you position your mouse near any icon the name will appear.) and the following menu will result. Notice that a red warning sign appears telling you what is required: "Requires a feed stream."
- 16) Fill out this menu as follows for the separator:
  - a) Name: Separator
  - b) Inlet: Feed (choose this stream by clicking on <<stream>> and then selecting from the drop down menu. (This saves time in typing stream names.)
  - c) Vapor Outlet: Vapor
  - d) Liquid Outlet: Liquid
  - e) Energy: Leave Blank for an insulated separator.



17) Your separator window should resemble the picture on Page 4. Notice that you have a green filled OK bar at the bottom of the screen. If you have filled in a name for the Energy stream, then there is a yellow warning for unknown heat duty. Go back and delete this stream. Close this window.

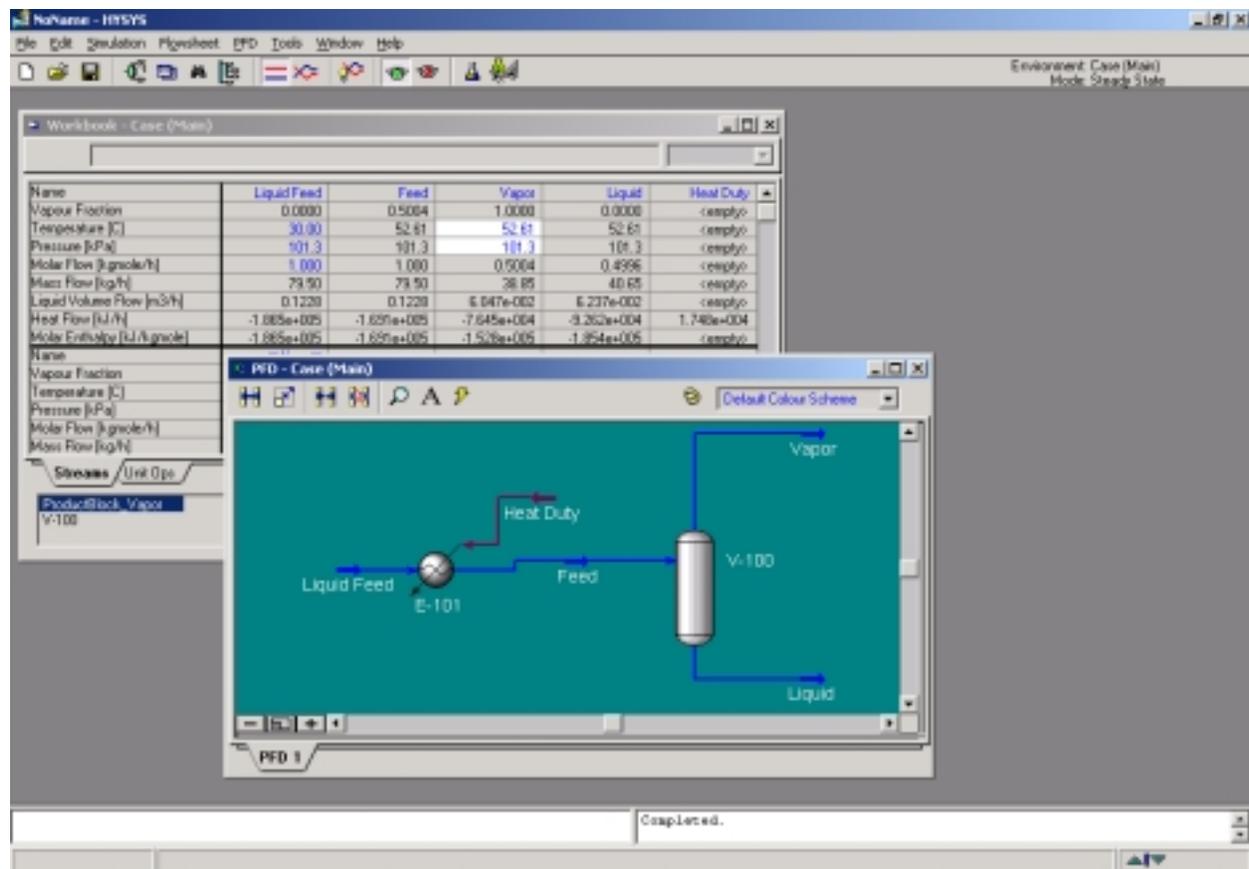
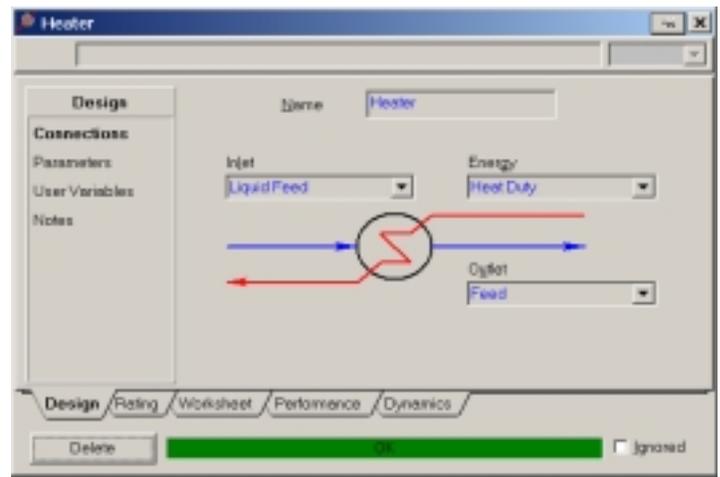
18) Next install a heater from the unit operations palette. The heater has the red-downward pointing arrow. Fill out this menu as follows for the separator:

- Name: Heater
- Inlet: Liquid Feed.
- Outlet: Feed (choose this stream by clicking on <<stream>> and then selecting from the drop down menu. (This saves time in typing stream names.)
- Energy: Heat Duty.

19) To change the specification of the Liquid Feed stream first delete the specifications in the Feed stream (Blue numbers.). Make the Liquid Feed stream a subcooled liquid by choosing a temperature less than the bubble point. What temperature must the feed be below to have only liquid present?  $T \leq$  \_\_\_\_\_

20) For the example below I will choose a Liquid Feed temperature of 30°C and a Liquid Feed pressure of 1 atm.

21) Next set vapor outlet stream temperature (Vapor) to get a vapor fraction of 0.5 (the pressure should be kept at 1 atm) What is the resulting temperature for a 50 % vap-liq mixture?  $T \cong$



Click on the Work Sheet tab and you will see that an isothermal flash has been conducted. To determine the heat duty you must select the Energy Streams tab. For this flash the heat duty is 17,700 kJ/hr.

- 22) Now the real question that all of you are asking is why is this called an isothermal flash? An isothermal flash is defined as fully specifying a feed stream ( $T_F$ ,  $P_F$ , and *compositions*) and the temperature and pressure of one outlet stream. Remember that the above simulation was obtained by deleting specifications. If you over specify the problem (variables > equations) HYSYS will give an error and go to a **stopped** mode. Fix the error by deleting specifications and press the **go** button (green traffic signal).
- 23) Printout your HYSYS workbook Specsheets and PFD. To print a specsheet:
- Check the printer by selecting File Printer Setup. The graphics printer prints the pfd's and the report printer prints text or workbook.
  - Select the workbook by pressing the toolbar button as shown in the figure below.
  - Select File, Print,
  - Choose All Pages - Compact.
  - Preview it

**Also printout your process flow diagram, (PFD) by choosing the print command while the PFD is active.**

### Adiabatic Flash

A common technique to perform a flash operation of a high pressure fluid is to release it to a low pressure through a valve. We will add a valve unit operation in this portion and set the Heat Duty to zero. A zero heat duty implies that there are no heat losses in the system. Once again in order to solve a single stage flash operation the typical variables specified are the feed stream, and 2 other variables. In the case of an adiabatic flash the variables are zero heat duty and the outlet stream pressure.

- 24) Before adding these streams delete the specifications to temperature and pressure in the feed stream and the vapor stream. If you ever get to a situation that HYSYS stops calculating values, it is because you have an inconsistency error. HYSYS tells you when it has **stopped** calculating values (holding mode) when the **GO** icon (stop light signal) is present. To have HYSYS start calculating again you must fix your error and then press the **GO** icon to toggle to the automatic calculation mode. Currently the separator unit operation is adiabatic, since no stream name was provided for the energy stream within the separator unit operation. (If a stream name was provided then the separator energy stream must be specified as zero. This will change the color of these numbers to blue.)

- 25) Delete the heater and add the valve by double clicking on the valve icon in the unit operation palette (press F4 to show).

- 26) Label the feed to the valve "high pressure liquid" and connect the outlet of the valve to the feed. Specify "high pressure liquid" to have a pressure of 10 atm and temperature of 118°C. Check to make sure that you have a liquid below its bubble point. Determine the bubble point temperature of this "high pressure liquid" stream at 10 atm.  $T =$

Name	High Pressure L	Feed	Liquid	Vapor
Vapour Fraction	0.0000	0.4990	0.0000	1.0000
Temperature [C]	118.0	53.45	53.45	53.45
Pressure [kPa]	1013	101.3	101.3	101.3
Molar Flow [kgmole/h]	1.000	1.000	0.5010	0.4990
Mass Flow [kg/h]	79.87	79.87	40.94	38.93
Liquid Volume Flow [m3/h]	0.1233	0.1233	6.274e-002	6.051e-002
Heat Flow [kJ/h]	-1.695e+005	-1.695e+005	-9.312e+004	-7.649e+004

Separator		
Separator Type		
Vessel Temperature	53.45	C
Vessel Pressure	101.3	kPa
Liquid Molar Flow	0.5010	kgmole/h
Duty	0.0000	kJ/h

27) The valve is based on the assumption that change of enthalpy of the stream is zero (Isenthalpic). Set the outlet pressure of the valve or product stream of the separator to give a vapor fraction of 0.5.  $P_{FEED} =$

What is the temperature of the feed to the separator?  $T_{FEED} =$  \_\_\_\_\_

Why is it so cold compared to the High Pressure Liquid feed to the valve?

28) Add a summary table to your unit operations by right clicking on a unit operation and selecting Show Table. Note that the "Heat Duty" on the separator is shown in the table as zero – which is adiabatic.

29) Printout your HYSYS workbook Specsheets and PFD. To print a specsheet:

30) Check the printer by selecting File Printer Setup. The graphics printer prints the pfd's and the report printer prints text or workbook.

a) Select the workbook by pressing the toolbar button as shown in the figure below

b) Select File, Print,

c) Choose All Pages - Compact.

d) Preview it and then print

**Also printout your process flow diagram, (PFD) by choosing the print command while the PFD is active.**

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