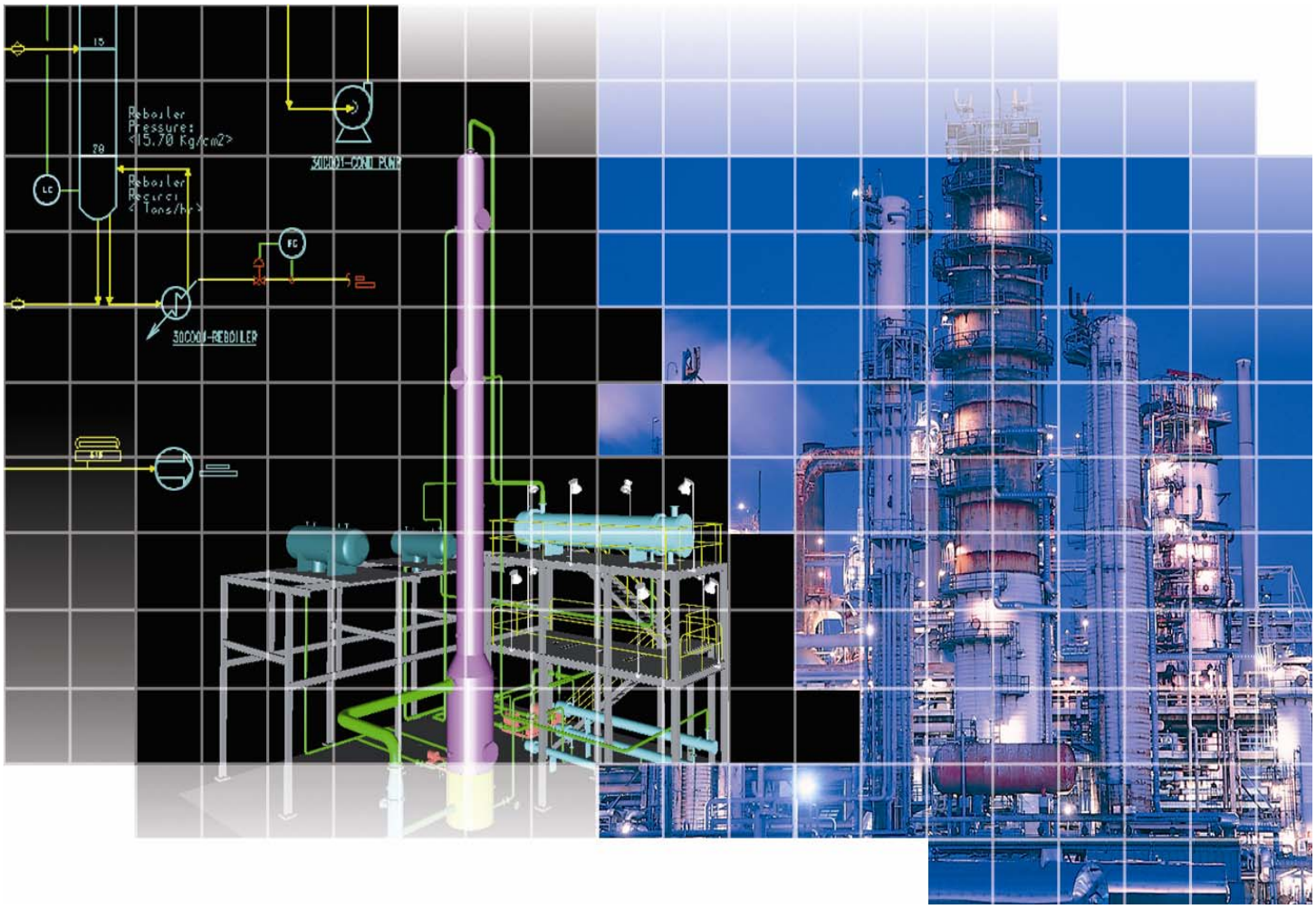

HYSYS®: An Introduction to Chemical Engineering Simulation

For UTM Degree++ Program

Mohd. Kamaruddin Abd Hamid

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Preface

HYSYS is a powerful engineering simulation tool, has been uniquely created with respect to the program architecture, interface design, engineering capabilities, and interactive operation. The integrated steady state and dynamic modeling capabilities, where the same model can be evaluated from either perspective with full sharing of process information, represent a significant advancement in the engineering software industry.

The various components that comprise HYSYS provide an extremely powerful approach to steady state modeling. At a fundamental level, the comprehensive selection of operations and property methods allows you to model a wide range of processes with confidence. Perhaps even more important is how the HYSYS approach to modeling maximizes your return on simulation time through increased process understanding.

To comprehend why HYSYS is such a powerful engineering simulation tool, you need look no further than its strong thermodynamic foundation. The inherent flexibility contributed through its design, combined with the unparalleled accuracy and robustness provided by its property package calculations leads to the presentation of a more realistic model.

HYSYS is widely used in universities and colleges in introductory and advanced courses especially in chemical engineering. In industry the software is used in research, development, modeling and design. HYSYS serves as the engineering platform for modeling processes from Upsteam, through Gas Processing and Cryogenic facilities, to Refining and Chemicals processes.

There are several key aspects of HYSYS which have been designed specifically to maximize the engineer's efficiency in using simulation technology. Usability and efficiency are two obvious attributes, which HYSYS has and continues to excel at. The single model concept is key not only to the individual engineer's efficiency, but to the efficiency of an organization.

Books about HYSYS are sometimes difficult to find. HYSYS has been used for research and development in universities and colleges for many years. In the last few years, however, HYSYS is being introduced to universities and colleges students as the first (and sometimes the only) computer simulator they learn. For these students there is a need for a book that teaches HYSYS assuming no prior experience in computer simulation.

The Purpose of this Book

HYSYS: An Introduction to Chemical Engineering Simulations is intended for students who are using HYSYS for the first time and have little or no experience in computer simulation. It can be used as a textbook in freshmen chemical engineering courses, or workshops where HYSYS is being taught. The book can also serve as a reference in more advanced chemical engineering courses when HYSYS is used as a tool for simulation and solving problems. It also can be used for self study of HYSYS by students and practicing engineers. In addition, the book can be a supplement or a secondary book in courses where HYSYS is used, but the instructor does not have time to cover it extensively.

Topics Covered

HYSYS is a huge and complex simulator, therefore it is impossible to cover all of it in one book. This book focuses primarily on the fundamental of HYSYS. It is believed that once these foundations are well understood, the student will be able to learn advanced topics easily by using the information in the Help menu.

The order in which the topics are presented in this book was chosen carefully, based on several years of experience in teaching HYSYS in an introductory chemical engineering course. The topics are presented in an order that allows the students to follow the book chapter after chapter. Every topic is presented completely in one place and then is used in the following chapters.

Software and Hardware

The HYSYS program, like most other software, is continually being developed and new versions are released frequently. This book covers HYSYS, Version 2004.1. It should be emphasized, however, that this book covers the basics of HYSYS which do not change that much from version to version. The book covers the use of HYSYS on computers that use the Windows operating system. It is assumed that the software is installed on the computer, and the user has basic knowledge of operating the computer.

ENGR. MOHD. KAMARUDDIN ABD. HAMID
Skudai, May 2007

Chapter 1
Starting with HYSYS

Starting with HYSYS

This chapter begins by starting HYSYS and how to select the right components and fluid package for simulation purposes. Knowing how to start HYSYS and get familiar with its desktop is very important in this chapter. The second part is about how to enter and re-enter the simulation environment, and get familiar with simulation flowsheet. In this part, users will be informed some important features of HYSYS. The last part is dealing with how to add and specify material streams for simulation. Variables specification is one of the important steps that users need to understand when dealing with HYSYS.

Learning Outcomes: At the end of this chapter, the user will be able to:

- Start HYSYS
- Select Components
- Define and select a Fluid Package
- Enter and re-enter Simulation Environment
- Add and specify material streams

1.1 Starting HYSYS

The installation process creates the following shortcut to HYSYS:

1. Click on the **Start** menu.
2. Select **Programs | AspenTech | Aspen Engineering Suite | Aspen HYSYS 2004.1 | Aspen HYSYS 2004.1**.

   The HYSYS Desktop appears:

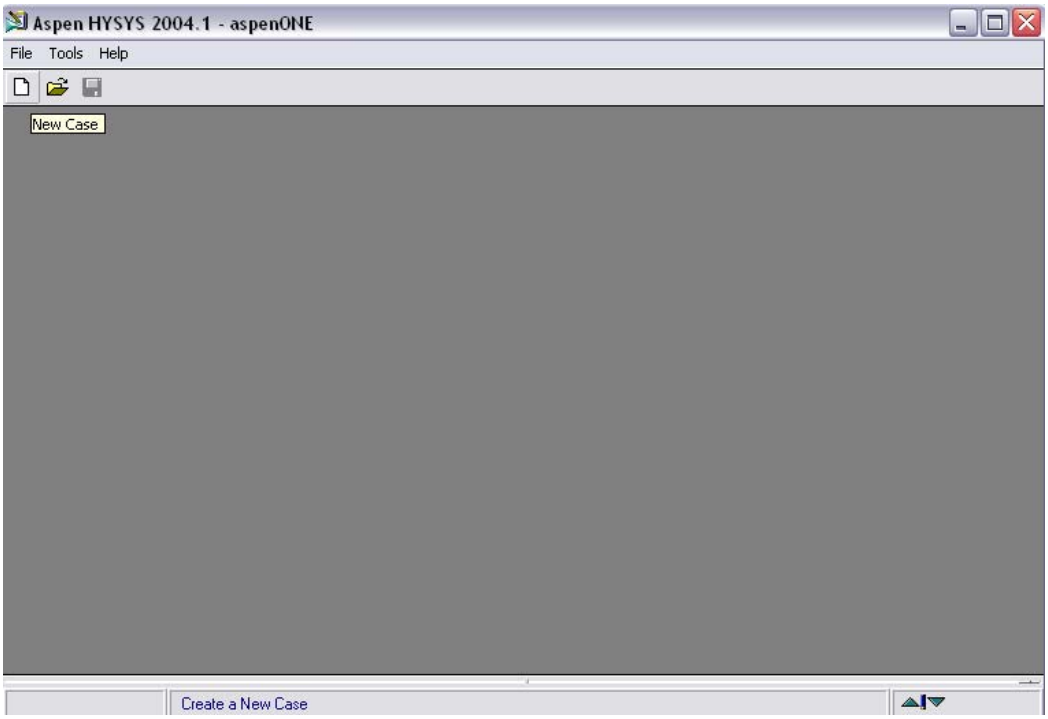


Figure 1-1

Before any simulation can occur, HYSYS needs to undergo an initial setup. During an initial setup, the components and the fluids package that will be used will be selected.

1.2 Simulation Basis Manager

Aspen HYSYS used the concept of the fluid package to contain all necessary information for performing flash and physical property calculations. This approach allows you to define all information (property package, components, hypothetical components, interaction parameters, reactions, tabular data, etc.) inside a single entity.

There are four key advantages to this approach:

- All associated information is defined in a single location, allowing for easy creation and modification of the information.
- Fluid packages can be stored as completely defined entities for use in any simulation.
- Component lists can be stored out separately from the Fluid Packages as completely defined entities for use in any simulation.

- Multiple Fluid Packages can be used in the same simulation. However, they are defined inside the common Basis Manager.

The Simulation Basis Manager is property view that allows you to create and manipulate multiple fluid packages or component lists in the simulation.

1.3 Creating A New Simulation

Select **File/New/Case** or press **Crtl+N** or click on the **New Case**  to start a new case. In HYSYS, your simulation is referred to as a "case". This will open up the **Simulation Basis Manager** which is where all of the components and their properties can be specified.

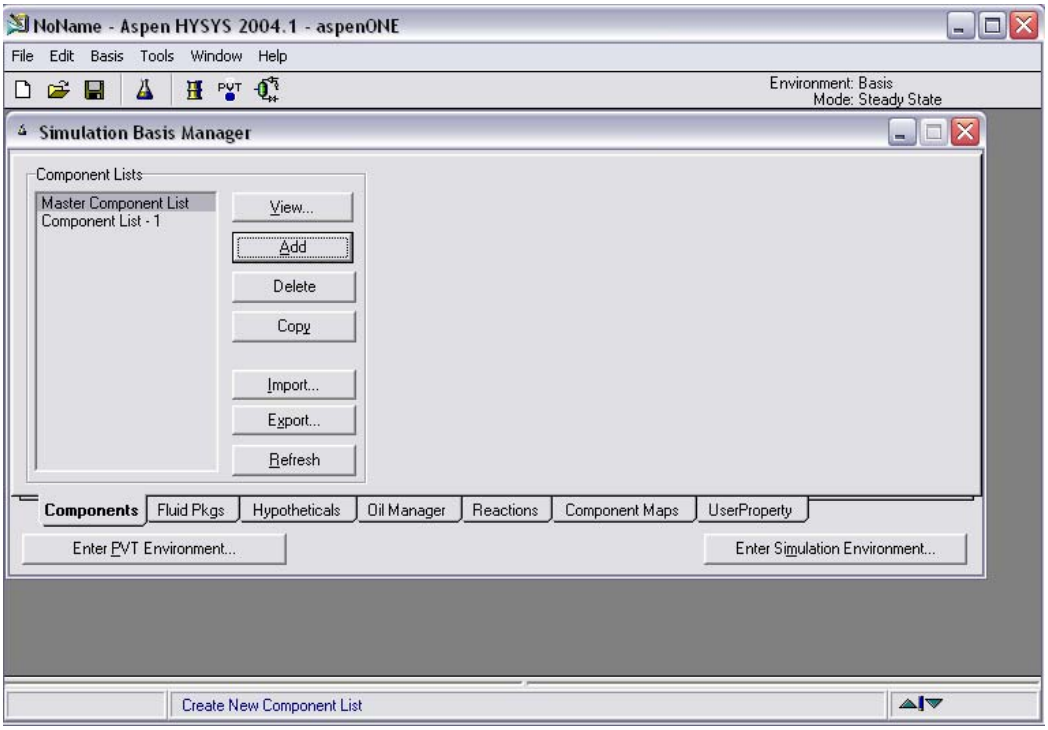


Figure 1-2

Saving Your Simulation

Before proceeding any further, save your file in an appropriate location. Select **File/Save As** and select where to save the file. **Do not** save the file to the default location.

1.4 Adding Components To The Simulation

The first step in establishing the simulation basis is to set the chemical components which will be present in your simulation.

1. To add components to the simulation, click on the **Add** button in the Simulation Basis Manager.
2. Clicking on **Add** will bring up the **Component List View** which is a list of all the components available in HYSYS.

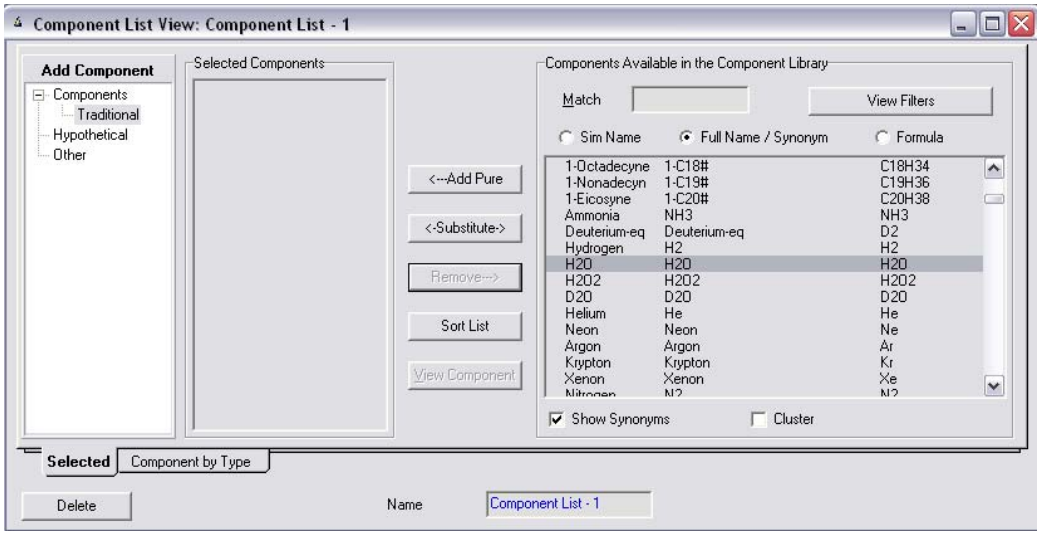


Figure 1-3

3. Select the desired components for your simulation. You can search through the list of components in one of three ways:

    a. Sim Name
    b. Full Name
    c. Formula

    Select which match term you want of the three above types by selecting the corresponding button above the list of components. Then type in the name of the component you are looking for. For example, typing in **water** for a Sim Name narrows the list down to a single component. If your search attempt does not yield the desired component, then either try another name or try searching under full name or formula.
4. Once you have located the desired component, either **double click** on the component or click **<---Add Pure** to add it to the list of components for the simulation.
5. At the bottom of the components page, you can give your component list a name.
6. Once this is complete, simply close the window by clicking the **red X** at the upper right hand corner of the component list view, which will return you to the simulation basis manager.

1.5 Selecting A Fluids Package

Once you have specified the components present in your simulation, you can now set the fluid package for your simulation. The fluid package is used to calculate the fluid/thermodynamic properties of the components and mixtures in your simulation (such as enthalpy, entropy, density, vapour-liquid equilibrium etc.). Therefore, it is very important that you select the correct fluid package since this forms the basis for the results returned by your simulation.

1. From the simulation basis manager (Figure 1-2), select the **Fluid Pkgs** tab.
2. Click the **Add** button to create a new fluid package as shown below:

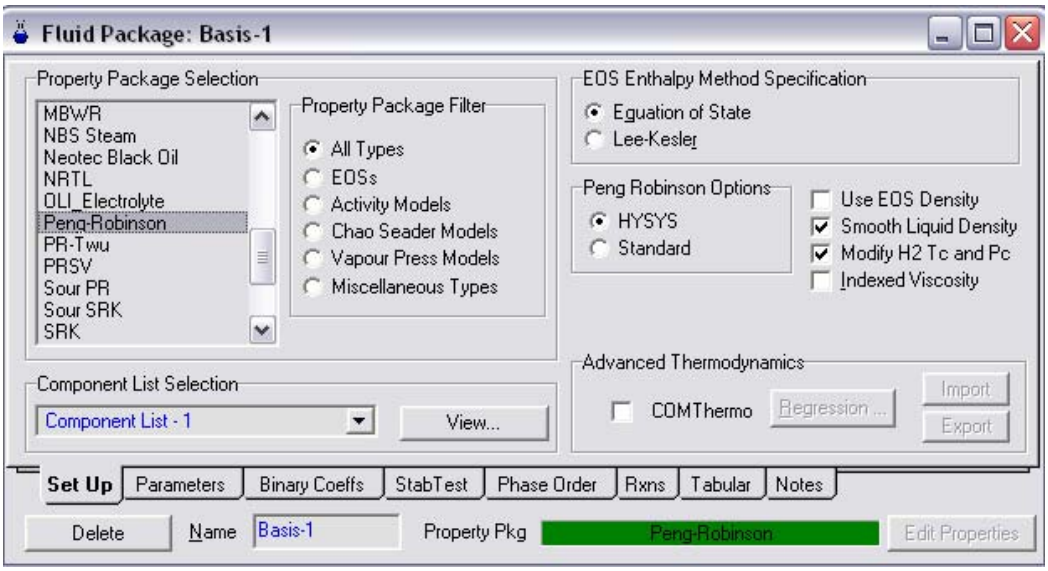


Figure 1-4

3. From the list of fluid packages, select the desired thermodynamic package. The list of available packages can be narrowed by selecting a filter to the left of the list (such as EOSs, activity models etc.).
4. Once the desired model has been located, select it by clicking on it once (no need to double click). For example, select **Peng-Robinson** property package for your simulation.
5. You can give your fluid package a name at the bottom of the fluid package screen (e.g. the name in Figure 1-4 is **Basis-1**).
6. Once this is done, close the window by clicking on the **red X** on the upper right hand corner of the Fluid Packages window.

1.6 Selecting Thermodynamics Model

When faced with choosing a thermodynamic model, it is helpful to at least a logical procedure for deciding which model to try first. Elliott and Lira (1999)[1] suggested a decision tree as shown in Figure 1-5.

The property packages available in HYSYS allow you to predict properties of mixtures ranging from well defined light hydrocarbon systems to complex oil mixtures and highly non-ideal (non-electrolyte) chemical systems. HYSYS provides enhanced equations of state (**PR** and **PRSV**) for rigorous treatment of hydrocarbon systems; semiempirical and vapor pressure models for the heavier hydrocarbon systems; steam correlations for accurate steam property predictions; and activity coefficient models for chemical systems. All of these equations have their own inherent limitations and you are encouraged to become more familiar with the application of each equation.

[1] Elliott and Lira, "Introduction to Chemical Engineering Thermodynamics", Prentice Hall, 1999.

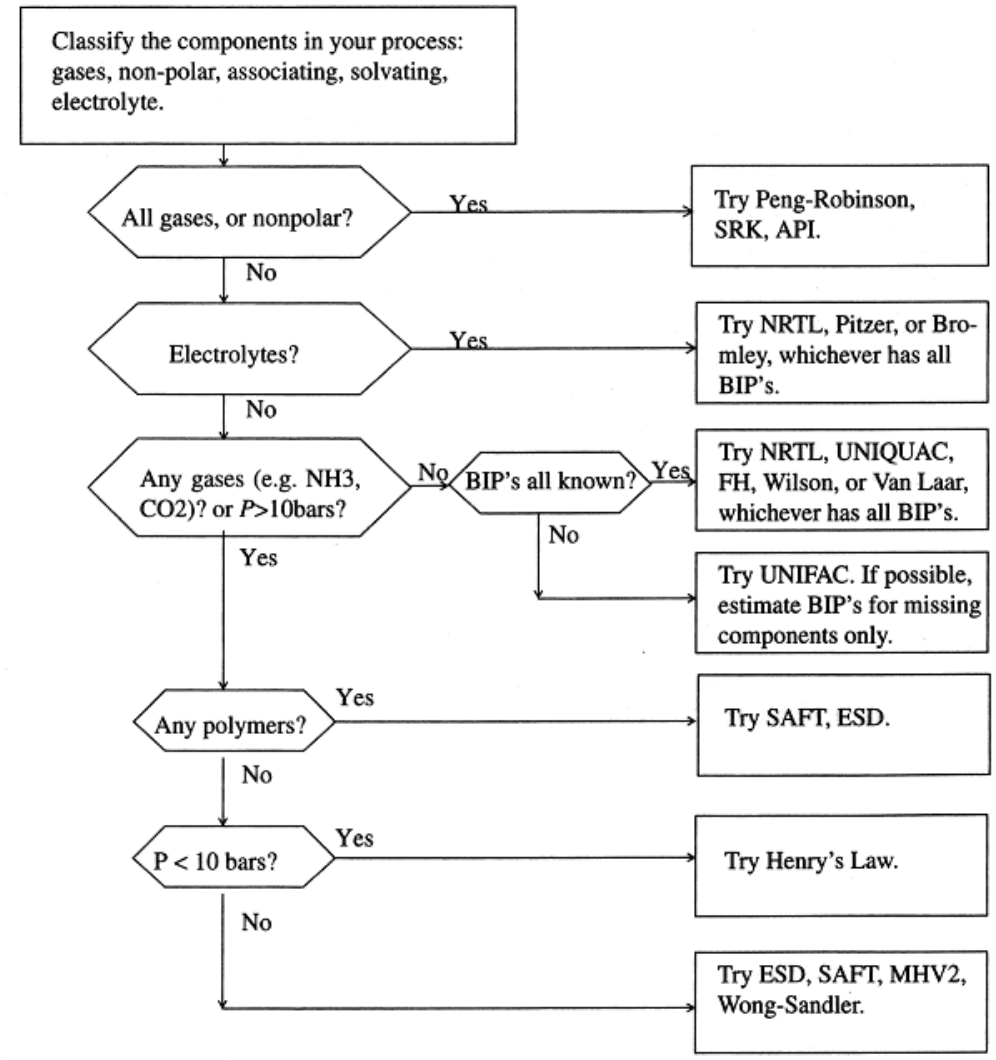


Figure 1-5

The following table lists some typical systems and recommended correlations.

Type of System	Recommended Property Method
TEG Dehydration	PR
Sour Water	PR, Sour PR
Cryogenic Gas Processing	PR, PRSV
Air Separation	PR, PRSV
Atm. Crude Towers	PR, PR Options, GS
Vacuum Towers	PR, PR Options, GS (<10 mmHg), Braun K10, Esso K
Ethylene Towers	Lee Kesler Plocker
High H_2 Systems	PR, ZJ or GS
Reservoir Systems	Steam Package, CS or GS
Hydrate Inhibition	PR
Chemical Systems	Activity Models, PRSV
HF Alkylation	PRSV, NRTL

Type of System	Recommended Property Method
TEG Dehydration with Aromatics	PR
Hydrocarbon systems where H_2O solubility in HC is important	Kabadi Danner
Systems with select gases and light HC	MBWR

PR=Peng-Robinson; PRSV=Peng-Robinson Stryjek-Vera; GS=Grayson-Streed; ZJ=Zudkevitch Joffee; CS=Chao-Seader; NRTL=Non-Random-Two-Liquid

For oil, gas and petrochemical applications, the Peng-Robinson EOS (**PR**) is generally the recommended property package. For more details, please refer Aspen HYSYS Simulation Basis Manual.

1.7 Enter Simulation Environment

You have now completed all necessary input to begin your simulation. Click on the **Enter Simulation Environment** button or click on the icon to begin your simulation as shown in Figure 1-6.

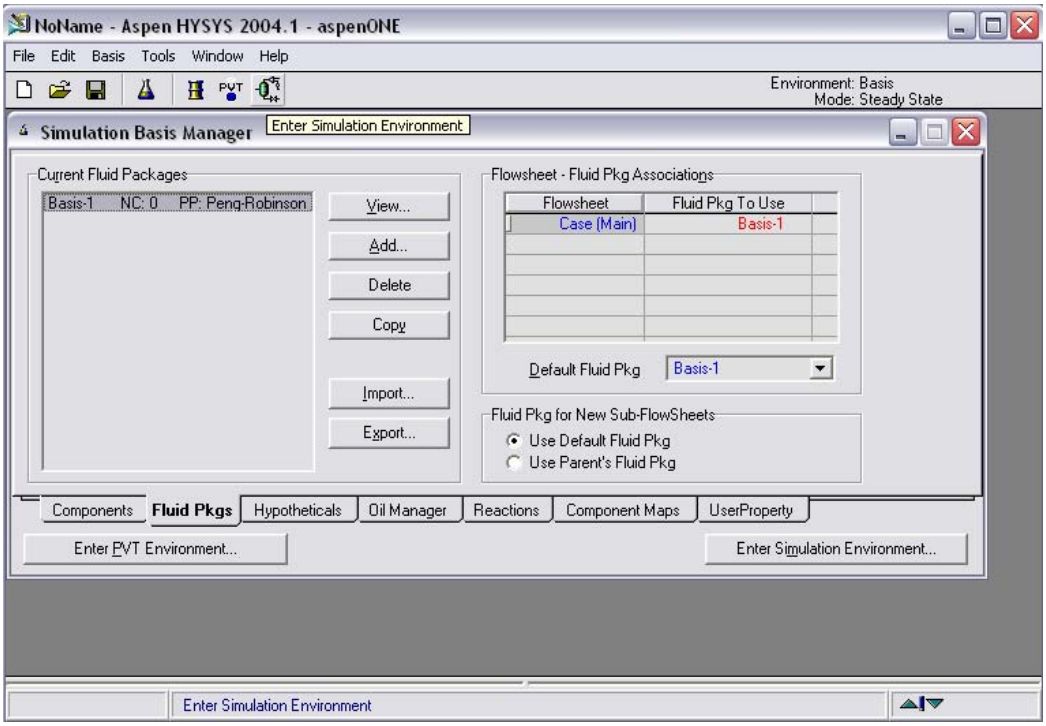


Figure 1-6

Working with Simulation Flowsheet

Once you have specified the components and fluid package, and entered the simulation environment, you will see the view as shown in Figure 1-7. Before proceeding, you should taking care of a few features of this simulation window:

1. HYSYS, unlike the majority of other simulation packages, solves the flowsheet after each addition/change to the flowsheet. This feature can be disabled by clicking the **Solver Holding** button (the **red** light button) located in the toolbar (see Figure 1-7). If this button is selected, then HYSYS will **not** solve the simulation and it will **not** provide any results. In order to allow HYSYS to return results, the **Solver Active** button (the **green** light button) must be selected.
2. Unlike most other process simulators, HYSYS is capable of solving for information both downstream and upstream. Therefore, it is very important to pay close attention to your flowsheet specification to ensure that you are not providing HYSYS with conflicting information. Otherwise, you will get an error and the simulation will **not** solve.

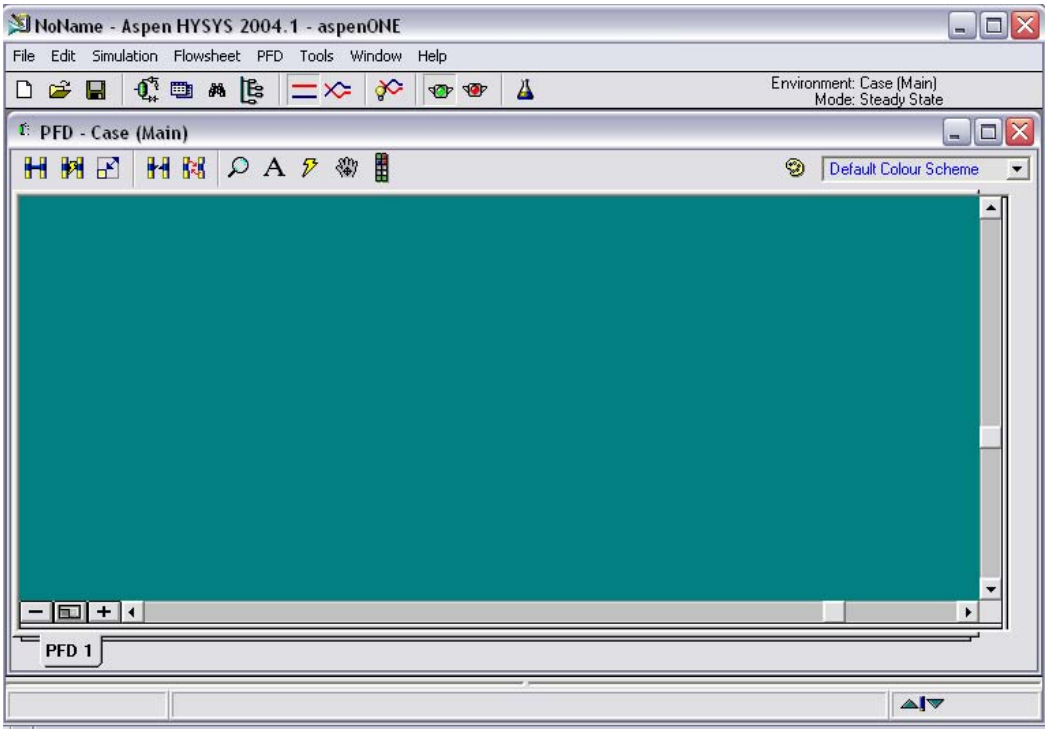


Figure 1-7

Re-Entering the Simulation Basis Manager

When the basis of the simulation has to be changed, the Simulation Basis Manager needs to be re-entered. Simply click on the icon on the top toolbar to re-enter it.

Accidentally Closing the PFD

Sometimes, people accidentally click the **red X** on the PFD. To get it back, simply go to **Tools –> PFDs**, make sure **Case** is selected, then click **View**.

Object Palette

On the right hand side of Figure 1-8, you will notice a vertical toolbar. This is known as the **Object Palette**. If for any reason this palette is **not** visible, got to the **Flowsheet** pulldown

menu and select **Palette** or press **F4** to display the palette. It is from this toolbar that you will add streams and unit operations to your simulation.

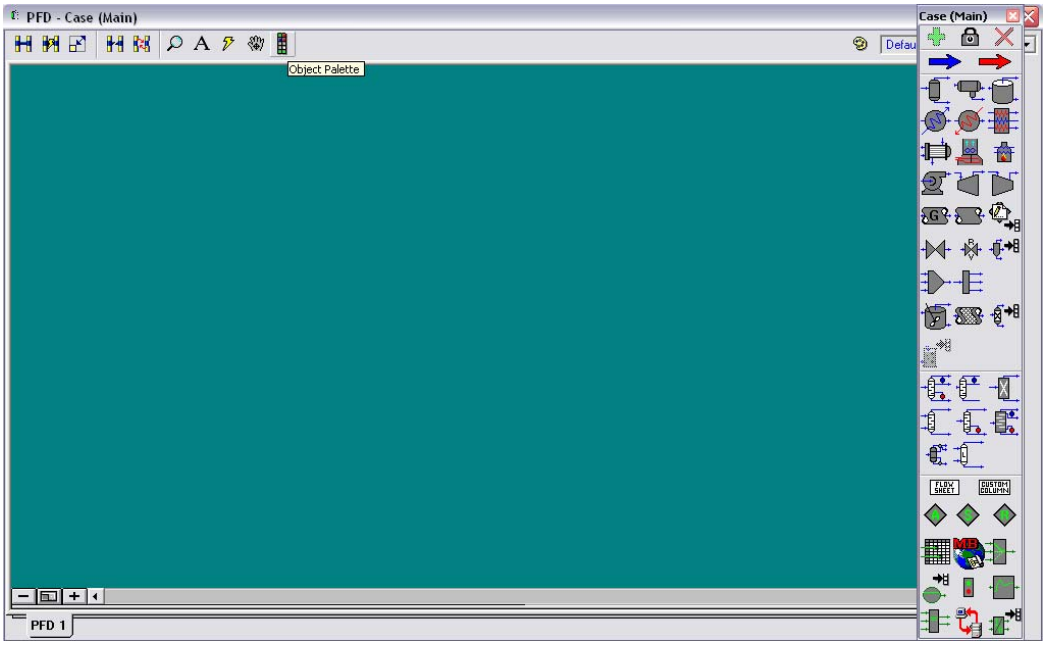


Figure 1-8

1.8 Adding Material Streams

Material Streams are used to transport the material components from process units in the simulation. A material stream can be added to the flowsheet in one of three ways:

1. Click on the blue arrow button on the Object Palette
2. Selecting the “Flowsheet” menu and selecting “Add Stream”
3. Pressing F11

Using any of the above methods will create a new material stream (a Blue arrow) on the flowsheet, refer Figure 1-9. The HYSYS default names the stream in increasing numerical order (i.e. the first stream created will be given the name “1”). This name can be modified at any time.

Specifying Material Streams

To enter information about the material stream, double click on the stream to show the window shown in Figure 1-10. It is within this window that the user specifies the details regarding the material stream. For material stream that will be used as an input, we need to specify **four** variables. Within HYSYS environment, input material stream always have four degree of freedoms. Meaning, we need to supply four information in order to fulfill the requirement for HYSYS to start its calculations.

> ***Tips:*** *Four variables needed for input stream are composition, flowrate, and two from temperature, pressure or vapor/phase fraction.*

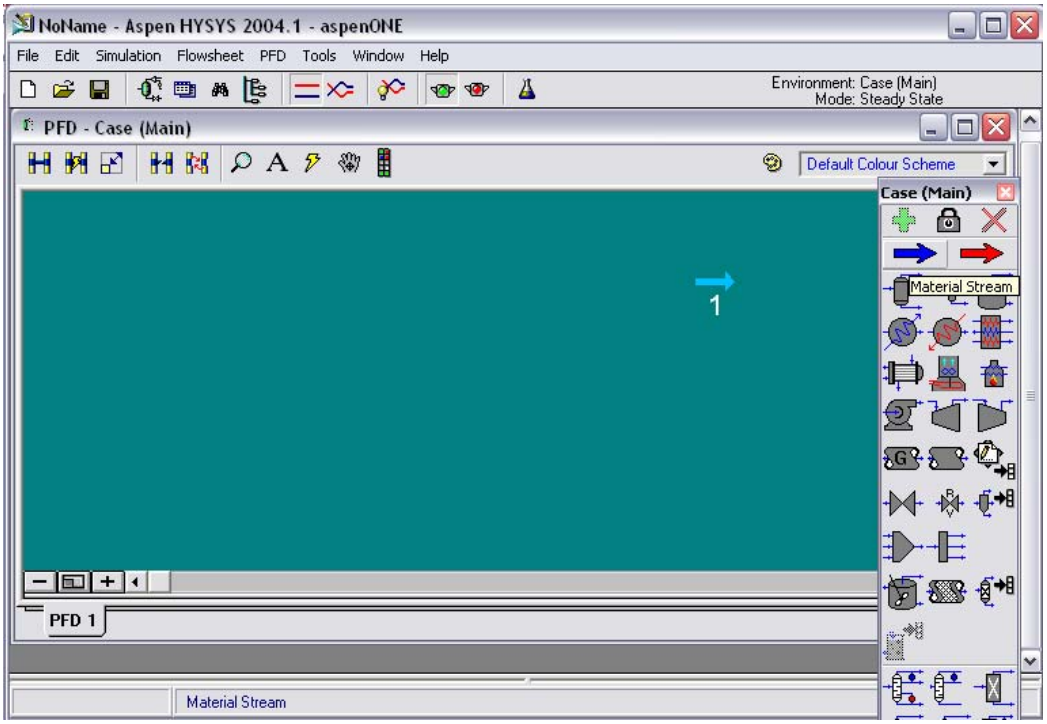


Figure 1-9

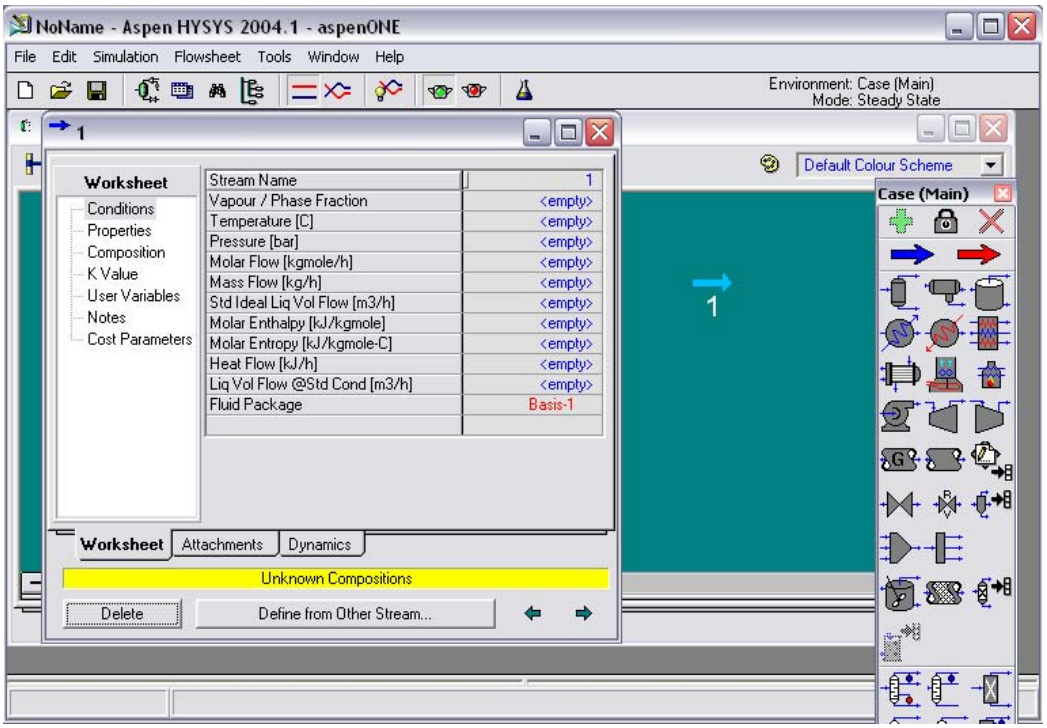


Figure 1-10

From Figure 1-10, you will see the warning yellow message bar at the bottom of the window indicating what information is needed (unknown compositions). Just follow what the message wants, for example, the first thing that you need to supply is compositions. In order to specify

the composition of the stream, select the “Composition” option from this list to display the window in Figure 1-11. It is within this window that the user specifies the composition of the stream. Note that only the components that you specified in the simulation basis manager will appear in this list. You can specify the composition in many different ways by clicking on the “Basis…” button. The HYSYS default is mole fractions, however the user can also specify mass fractions, liquid volume fractions, or flows of each component. If the user is specifying fractions, all fractions must add up to 1. Enter mole fraction of **1** in the H2O section to indicate 1 mole fraction of water.

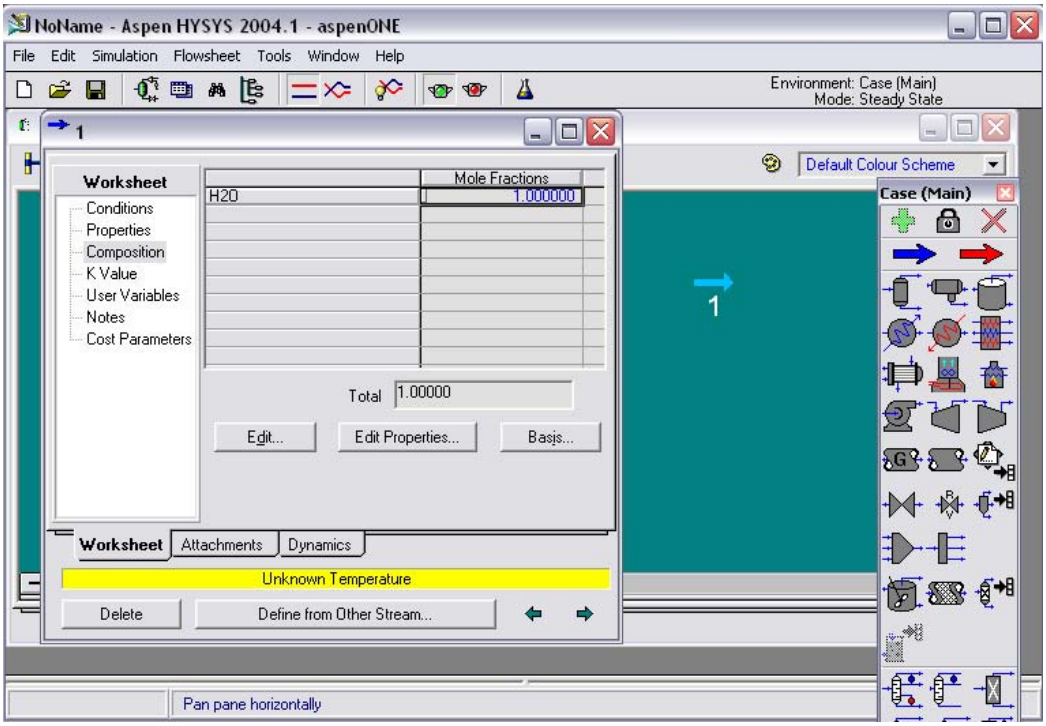


Figure 1-11

Next, the warning yellow message bar indicates that you need to specify the input temperature for this stream. In order to specify the temperature of the stream, select the “Conditions” option from this list to display the window in Figure 1-12. It is within this window that the user specifies the temperature of the stream.

When entering the conditions for a stream, it is not necessary to enter the values in the default units provided. When the user begins to enter a value in one of the cells, a drop down arrow appears in the units box next to the cell. By clicking on this drop down arrow, the user can specify any unit for the corresponding value and HYSYS will automatically convert the value to the default unit set. Enter the temperature of **25** in the temperature section to indicate the temperature of 25^{o}C. Next, the yellow warning message bar indicates that you need to specify the input pressure for this stream. In the same window, enter the pressure of **1** in the pressure section to indicate the pressure of 1 bar as shown in Figure 1-13.

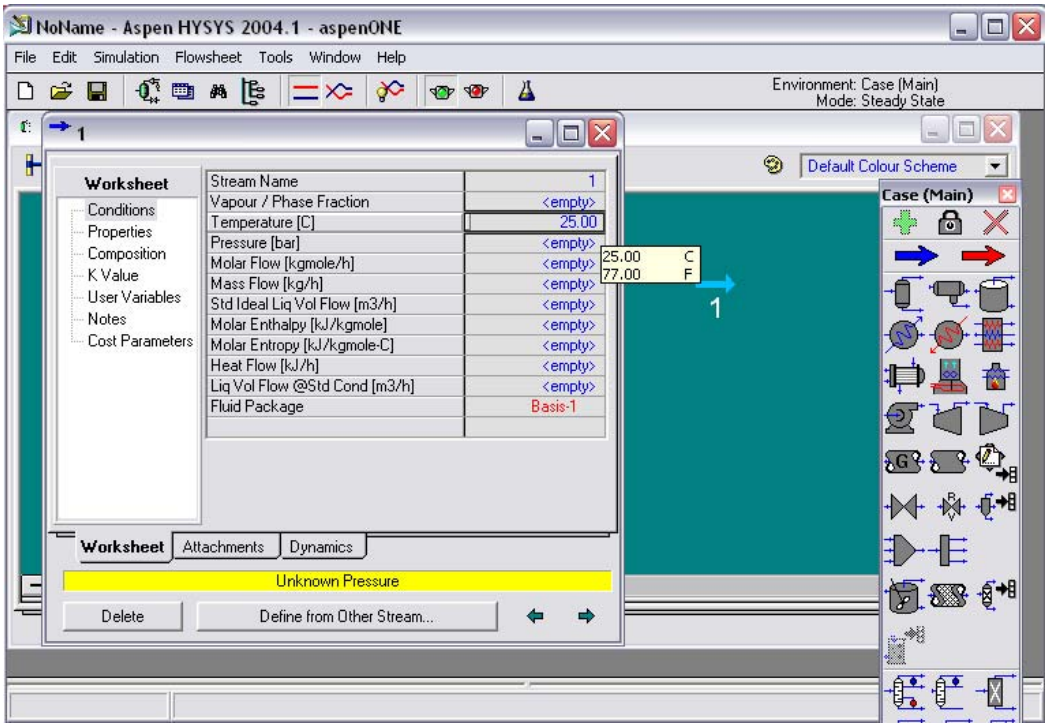


Figure 1-12

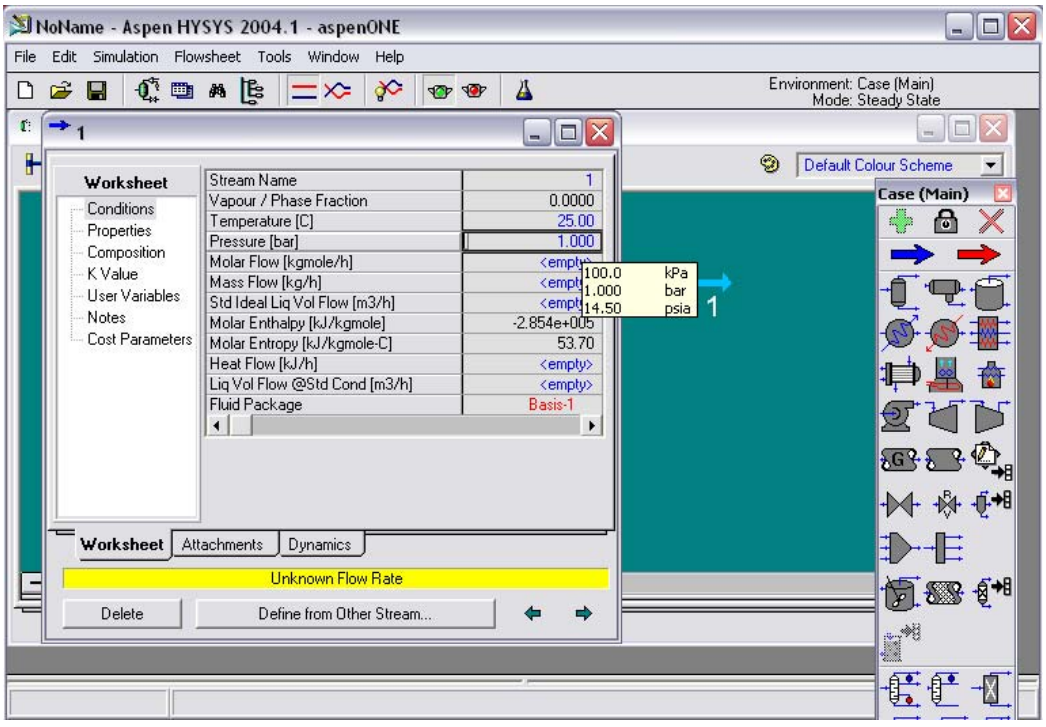


Figure 1-13

Next, the last variable that you need to specify is flowrate. For this, you have two options either to specify molar flowrate or mass flowrate. In the same window, enter the molar flowrate of **100** in the molar flowrate section to indicate the flowrate of 100 kgmole/h as shown in Figure 1-14.

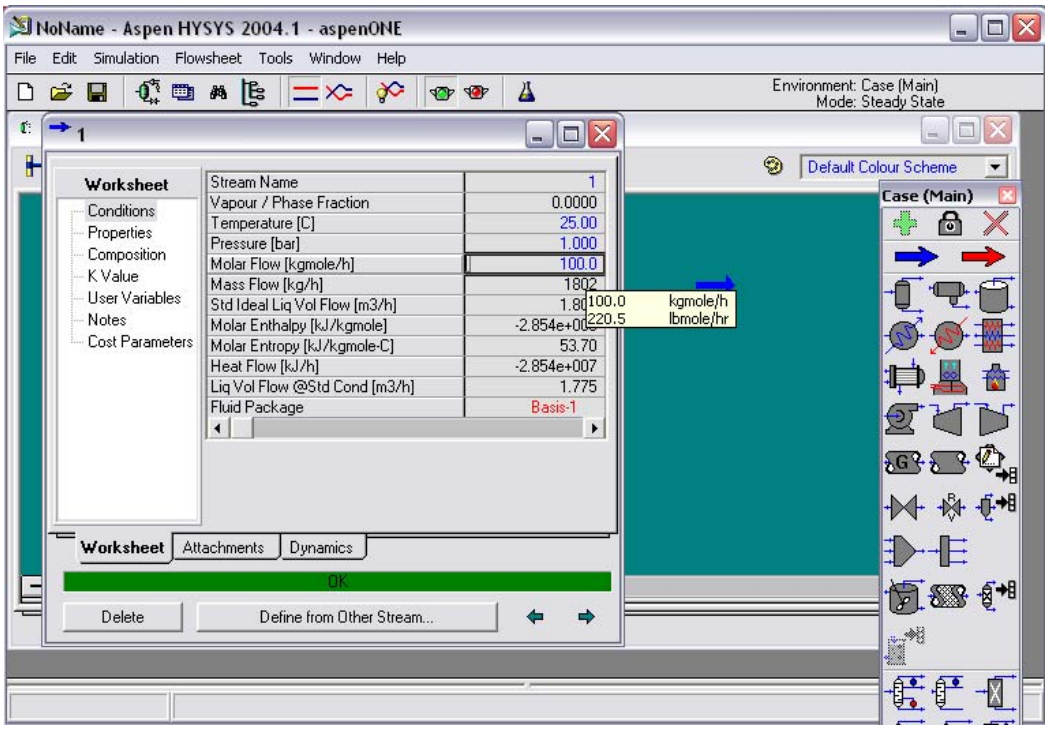


Figure 1-14: Input Stream Flowrate Specification

Once all of the stream information has been entered, HYSYS will calculate the remaining properties and data provided it has enough information from the rest of the flowsheet. Once a stream has enough information to be completely characterized, a green message bar appears at the bottom of the window within the stream input view indicating that everything is "OK" (See Figure 1-14). Otherwise, the input window will have a yellow message bar at the bottom of the window indicating what information is missing.

What is the Vapor/Phase Fraction of this stream? _____

Values shown in **blue** have been specified by the user and can be modified while values shown in **black** have been calculated by HYSYS and can not be modified. For example, in Figure 1-14 the temperature, pressure and molar flowrate have been specified while all other values shown have been calculated.

The following color code for material streams **on the flowhseet** indicates whether HYSYS has enough information to completely characterize the stream:

Royal Blue = properly specified and completely solved

Light blue = incompletely specified, properties **not** solved for

Therefore, if the arrow for the material stream is **royal blue**, then all of its properties have been calculated. At any time, the specifications and calculated properties for a stream can be viewed and modified by simply double clicking on the desired stream.

Save your case.

1.9 Review And Summary

In the first part of this chapter, we opened it with how to start HYSYS and get familiar with its desktop environment. We also discussed how to select components that will be used in simulation. Selecting the right fluid/thermodynamic package is very important and therefore we provided a flowchart that will assist users to select the right thermodynamics models.

The second part of this chapter was about how to enter and re-enter the simulation environment, and get familiar with simulation flowsheet. In this part, users are also informed some important features of HYSYS.

The last part of this chapter was dealing with how to add and specify material streams for simulation. Variables specification is one of the important steps that users need to understand when dealing with HYSYS. When users wanted to specify streams especially materials, they need to specify at least four variables in order to have HYSYS to calculate the remaining properties.

1.10 Problems

1.1. Create one materials stream that contains only water with following conditions:
- Fluid Package: Peng-Robinson
- Flowrate: 100 kgmole/h
- Pressure: 1 atm
- Vapor/Phase Fraction: 1.00

What is the temperature of this stream? _____

1.2. Repeat the above procedures by replacing pressure with temperature of 150^{o}C.

What is the pressure of this stream? _____

1.3. With the same condition in (2), reduce the temperature to 70^{o}C.

What is the new pressure of this stream? _____

1.4. Create one new materials stream that contains only water with following conditions:
- Fluid Package: Peng-Robinson
- Flowrate: 100 kgmole/h
- Pressure: 2 atm
- Vapor/Phase Fraction:1.00

What is the temperature of this stream? _____

1.5. With the same condition in (4), increase the pressure to 5 atm.

What is the new temperature of this stream? _____

1.6. With the same condition in (4), decrease the pressure to 0.5 atm.

What is the new temperature of this stream? _____

1.7. What can you conclude from these problems (1-6)?

_____

_____

_____

Chapter 2
Equation of State

Equation of State

Solving equations of state allows us to find the specific volume of a gaseous mixture of chemicals at a specified temperature and pressure. Without using equations of state, it would be virtually impossible for us to design a chemical plant. By knowing this specific volume, we can determine the size and thus the cost of the plant.

HYSYS currently offers the enhanced Peng-Robinson (PR) and Soave-Redlich-Kwong (SRK) equations of state. Of these, the Peng-Robinson equation of state supports the widest range of operating conditions and the greatest variety of systems. The Peng-Robinson and Soave-Redlich-Kwong equations of state generate all required equilibrium and thermodynamic properties directly.

The PR and SRK packages contain enhanced binary interaction parameters for all library hydrocarbon-hydrocarbon pairs (a combination of fitted and generated interaction parameters), as well as for most hydrocarbon-nonhydrocarbon binaries.

This chapter will guide you to determine the specific volume of a gaseous mixture of chemicals at a specified temperature and pressure. In addition, you will learn how to analyze the component property by using the Case Study utility.

Learning Outcomes: At the end of this chapter, the user will be able to:

- Determine the specific volume of a pure component or a mixture with HYSYS
- Compare the results obtained with different equations of state
- Preview the result using Workbook
- Analyze the property using Case Studies

Prerequisites: Before beginning this chapter, the users need to know how to:

- Start HYSYS
- Select components
- Define and select a fluid package
- Add and specify material streams

2.1 Equations Of State – Mathematical Formulations

The ideal gas equation of state, which relates the pressure, temperature, and specific volume, is a familiar equation:

$$pV = nRT \text{ or } p\hat{v} = RT \text{ where } \hat{v} = \frac{V}{n}$$

The term p is the absolute pressure, V is the volume, n is the number if moles, R is the gas constant, and T is the absolute temperature. The units of R have to be appropriate for the units chosen for the other variables. This equation is quite adequate when the pressure is low (such as one atmosphere). However, many chemical processes take place at very high pressure. Under these conditions, the ideal gas equation of state may not be valid representation of reality.

Other equations of states have been developed to address chemical processes at high pressure. The first generalization of the ideal gas law was the van der Waals equation of state:

$$p = \frac{RT}{\hat{v} - b} - \frac{a}{\hat{v}}$$

This extension is just a first step, however, because it will not be a good approximation at extremely high pressures. The Redlich-Kwong equation of state is a modification of van der Waal's equation of state, and then was modified further by Soave to give the Soave-Redlich-Kwong (SRK) equation of state, which is a common one in process simulators. Another variation of Redlich-Kwong equation of state is Peng-Robinson (PR) equation of state.

The following page provides a comparison of the formulation used in HYSYS for the SRK and PR equations of state.

	Soave-Redlich-Kwong	**Peng-Robinson**
	$P = \frac{RT}{\hat{v} - b} - \frac{a}{\hat{v}(\hat{v} + b)}$ $Z^3 - Z^2 + (A - B - B^2)Z - AB = 0$	$P = \frac{RT}{\hat{v} - b} - \frac{a}{\hat{v}(\hat{v} + b) + b(\hat{v} - b)}$ $Z^3 - (1 - B)Z^2 + (A - 2B - 3B^2)Z - (AB - B^2 - B^3) = 0$
where		
$b =$	$\sum_{i=1}^{N} x_i b_i$	$\sum_{i=1}^{N} x_i b_i$
$b_i =$	$0.08664 \frac{RTc_i}{Pc_i}$	$0.077796 \frac{RTc_i}{Pc_i}$
$a =$	$\sum_{i=1}^{N}\sum_{j=1}^{N} x_i x_j (a_i a_j)^{0.5}(1 - k_{ij})$	$\sum_{i=1}^{N}\sum_{j=1}^{N} x_i x_j (a_i a_j)^{0.5}(1 - k_{ij})$
$a_i =$	$a_{ci}\alpha_i$	$a_{ci}\alpha_i$
$a_{ci} =$	$0.42748 \frac{(RT_{ci})^2}{P_{ci}}$	$0.457235 \frac{(RT_{ci})^2}{P_{ci}}$
$\alpha_i^{0.5} =$	$1 + m_i(1 - T_{ri}^{0.5})$	$1 + m_i(1 - T_{ri}^{0.5})$
$m_i =$	$0.48 + 1.574\omega_i - 0.176\omega_i^2$	$0.37464 + 1.54226\omega_i - 0.26992\omega_i^2$

	Soave-Redlich-Kwong	Peng-Robinson
$A =$	$\frac{aP}{(RT)^2}$	$\frac{aP}{(RT)^2}$
$B =$	$\frac{bP}{RT}$	$\frac{bP}{RT}$

2.2 Building The Simulation

Problem: Find the specific volume of *n*-butane at 500 K and 18 atm using the following equation of state:

- Soave-Redlich-Kwong (SRK)
- Peng-Robinson (PR)

The first step in building any simulation is defining the fluid package. A brief review on how to define a fluid package and install streams is described below. *For a complete description, see the previous chapter (Chapter 1: Starting with HYSYS).*

Accessing HYSYS

To start HYSYS:

1. Click on the **Start** menu.
2. Select **Programs | AspenTech | Aspen Engineering Suite | Aspen HYSYS 2004.1 | Aspen HYSYS 2004.1**.

Open a new case by using one of the following:

1. Go to the **File** menu, select **New**, followed by **Case**, or
2. Press **Ctrl N**, or
3. Click the **New** icon on the toolbar.

Defining the Simulation Basis

1. Enter the following values in the specified fluid package view:

On this page…	Select…
Property Package	Soave-Redlich-Kwong (SRK)
Components	*n*-butane

2. Click the **Enter Simulation Environment** button when you are ready to start building the simulation.

Installing a Stream

There are several ways to create streams. (For complete description, see the previous chapter.)

- Press **F11**. The Stream property view appears, or
- Double-click the **Stream** icon in the **Object Palette**.

Defining Necessary Stream

Add a stream with the following values.

In this cell…	Enter…
Name	1
Temperature	500 K
Pressure	18 atm
Composition	n-C_4 – 100%
Molar Flow	100 kgmole/h

Saving

1. Go to the **File** menu.
2. Select **Save As**.
3. Give the HYSYS file the name **EOS SRK** then press the OK button.

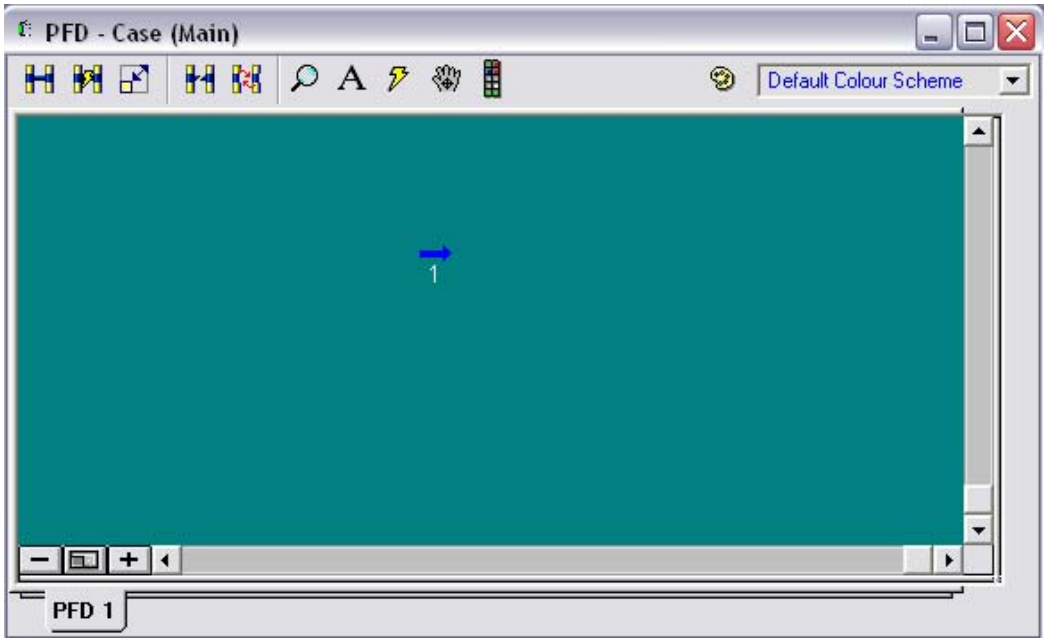


Figure 2-1

Preview the Result using Workbook

To preview the result for the simulation:

1. Go to the **Tools** menu and select **Workbooks** or click **Ctrl+W** as shown in Figure 2-2.
2. Next, click **View** and the Bookwork can be seen as shown in Figure 2-3.

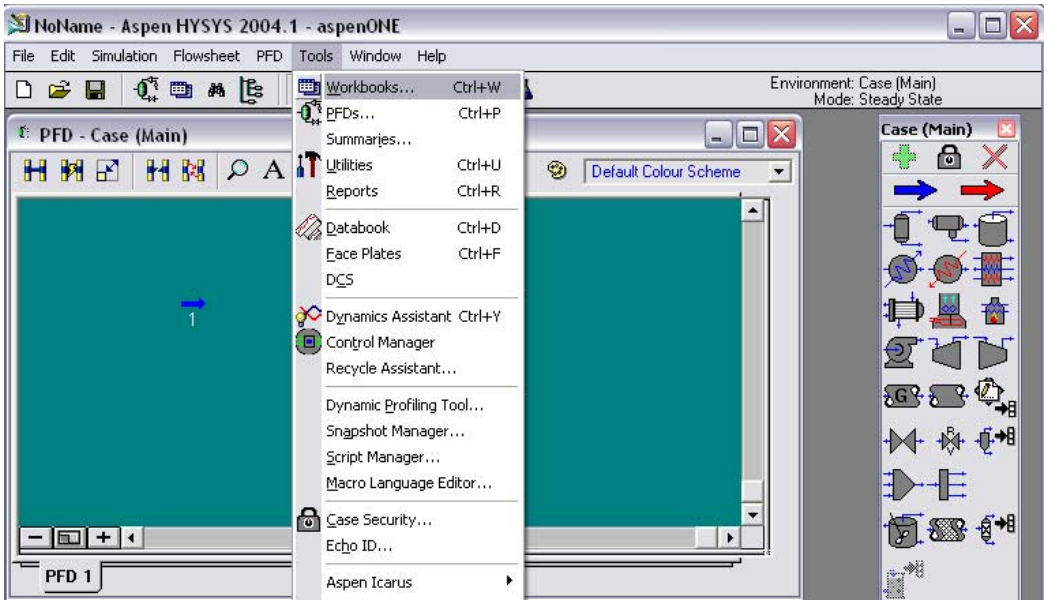


Figure 2-2

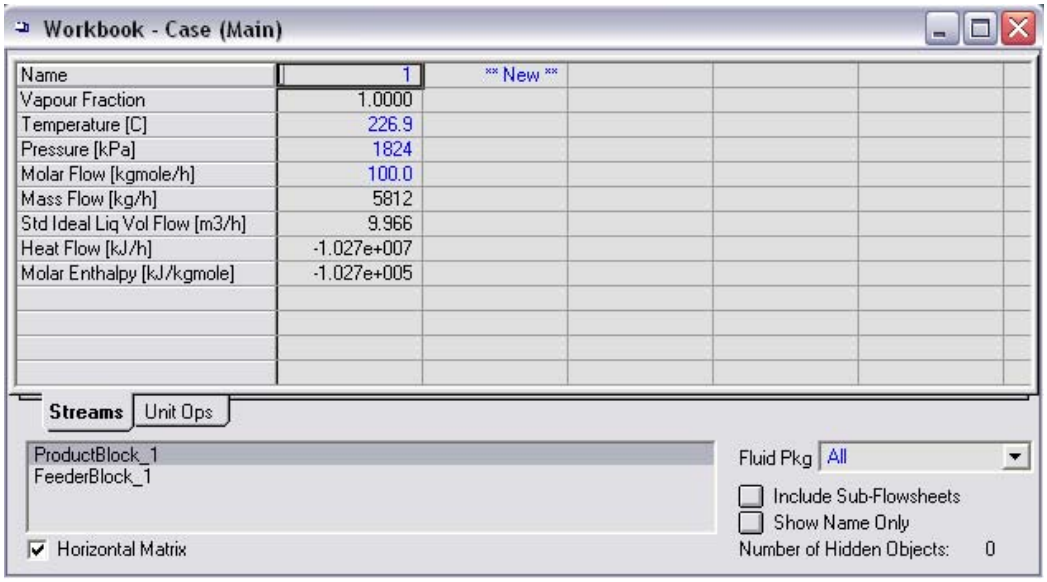


Figure 2-3

3. Specific volume in HYSYS is defined as Molar Volume. From Figure 2-3, there is no Molar Volume shown in the Workbook. In order to preview the value of Molar Volume, we have to add it to the Workbook.
4. To add the Molar Volume or other variables, go to the **Workbook** menu and click **Setup**. The setup window for Workbook can be viewed as shown in Figure 2-4.

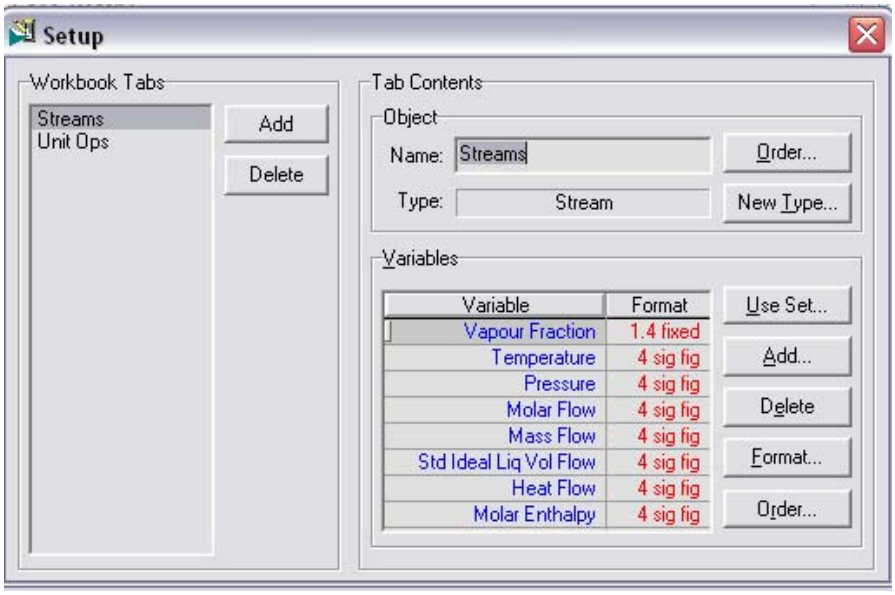


Figure 2-4

5. In the **Variables** tab, click the **Add** button at the right side of the window.
6. Window for you to select variables will appear as shown in Figure 2-5.

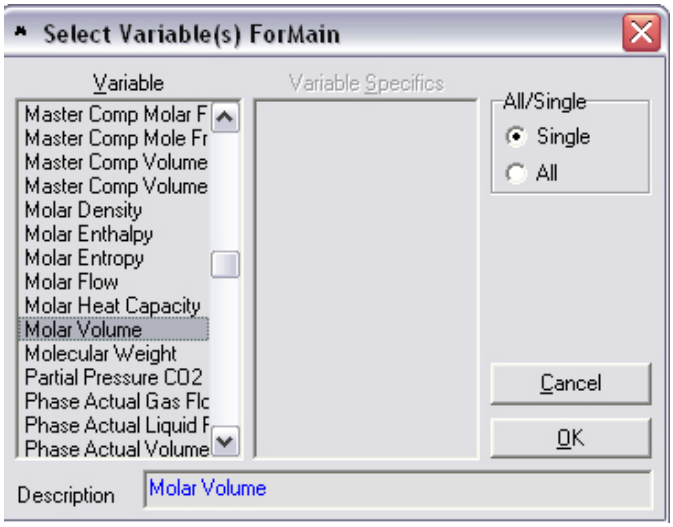


Figure 2-5

7. In the **Variable** tab, scroll down until you find the Molar Volume and then click **OK**. Close the Setup window by clicking the **red X** at the top right corner.
8. The Molar Volume value is presented in the Workbook as shown in Figure 2-6.

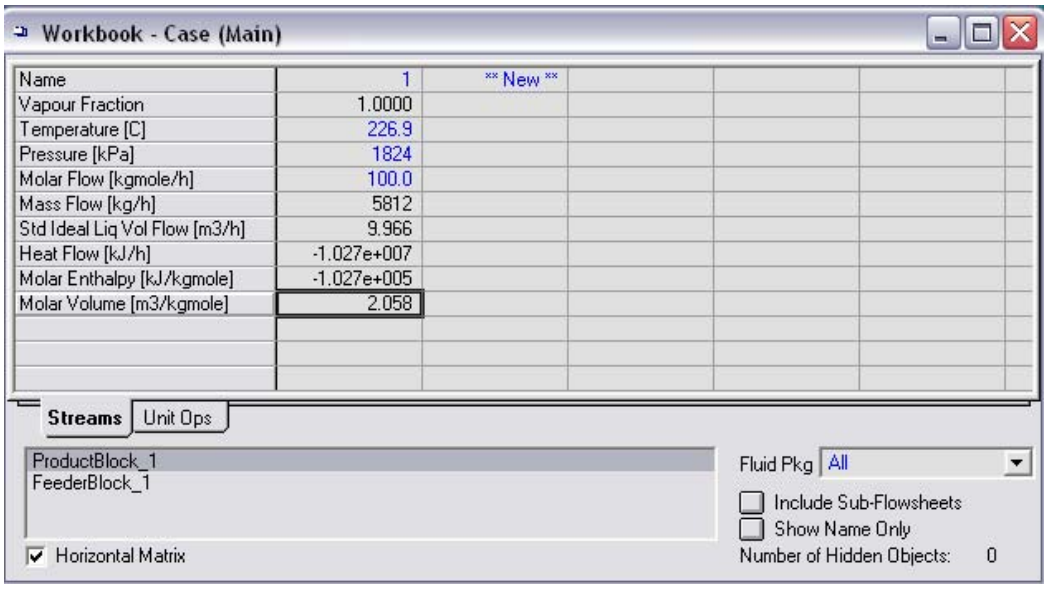


Figure 2-6

*What is the Molar Volume of n-butane?*_____

Analyze the Property using Case Study

In this section, we will analyze the specific volume of *n*-butane when the temperature is changing. To do this analysis, do the following:

1. Go to the **Tools** menu and select **Databook** or click **Ctrl+D** as shown in Figure 2-7.

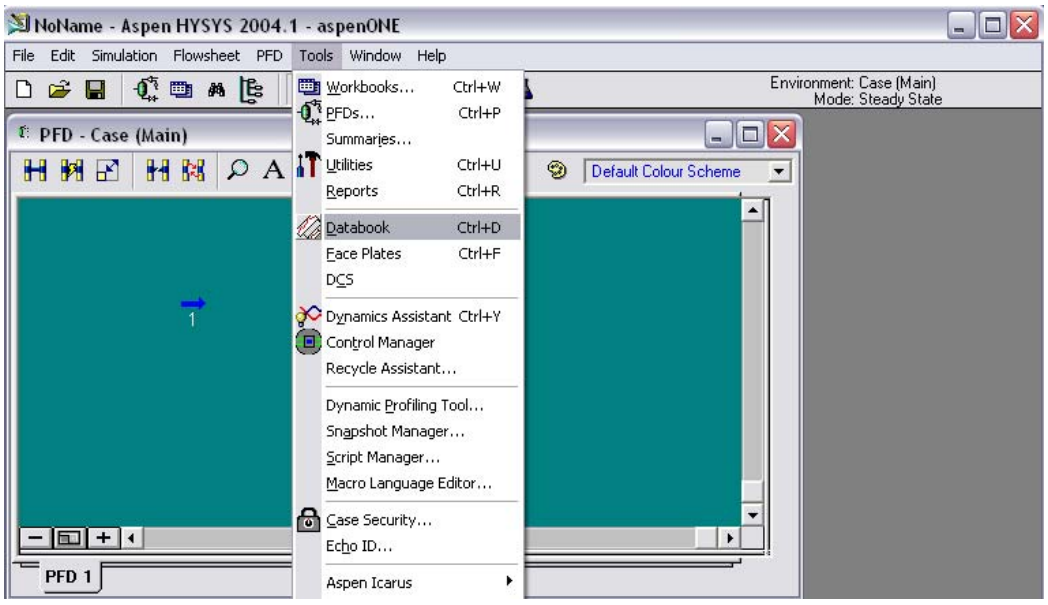


Figure 2-7

2. Next, click **Insert** button then **Variable Navigator** view displays as shown in Figure 2-8.

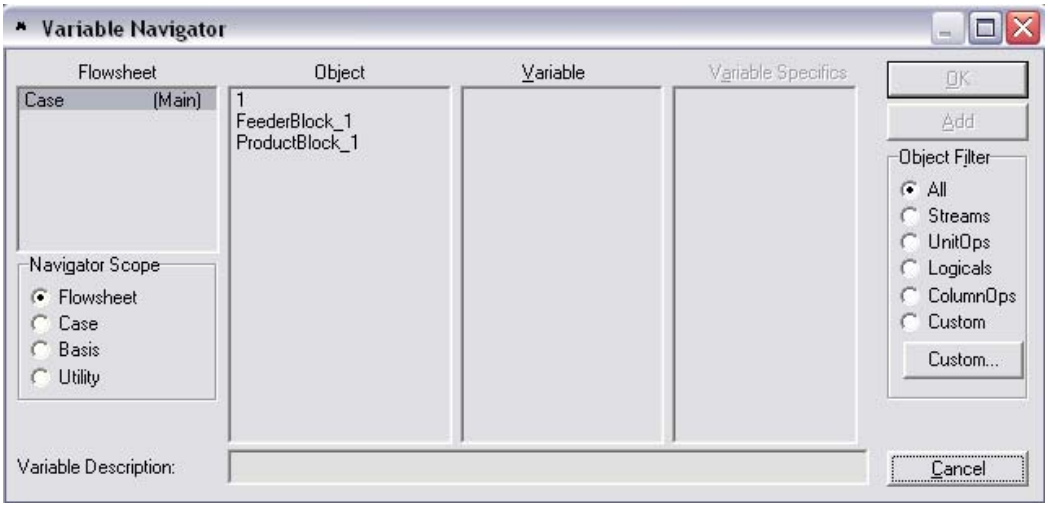


Figure 2-8

3. In the **Object** column, select stream 1, and in the **Variable** column, select Molar Volume. Then, click **OK** button.

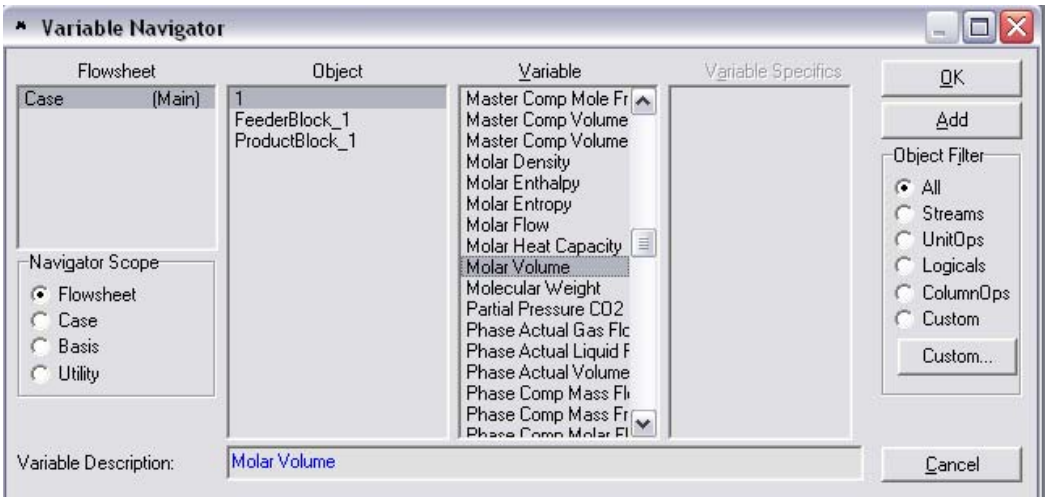


Figure 2-9

4. Repeat step 3 to insert **Temperature**. The new updated Databook is shown in Figure 2-10.

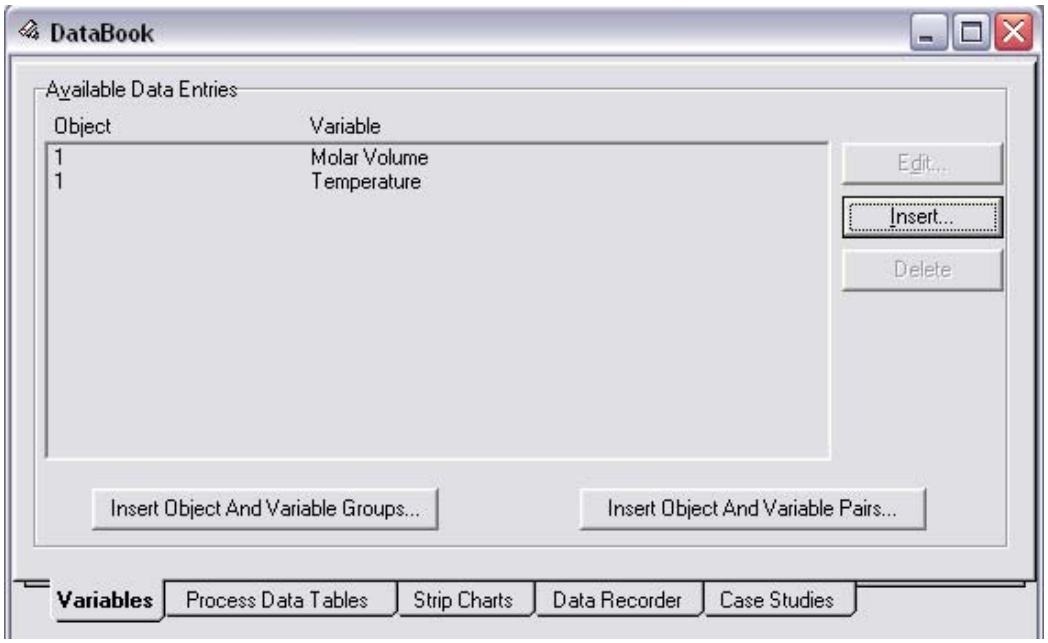


Figure 2-10

5. Switch to the Case Studies tab. Complete the tab as shown in the following figure.

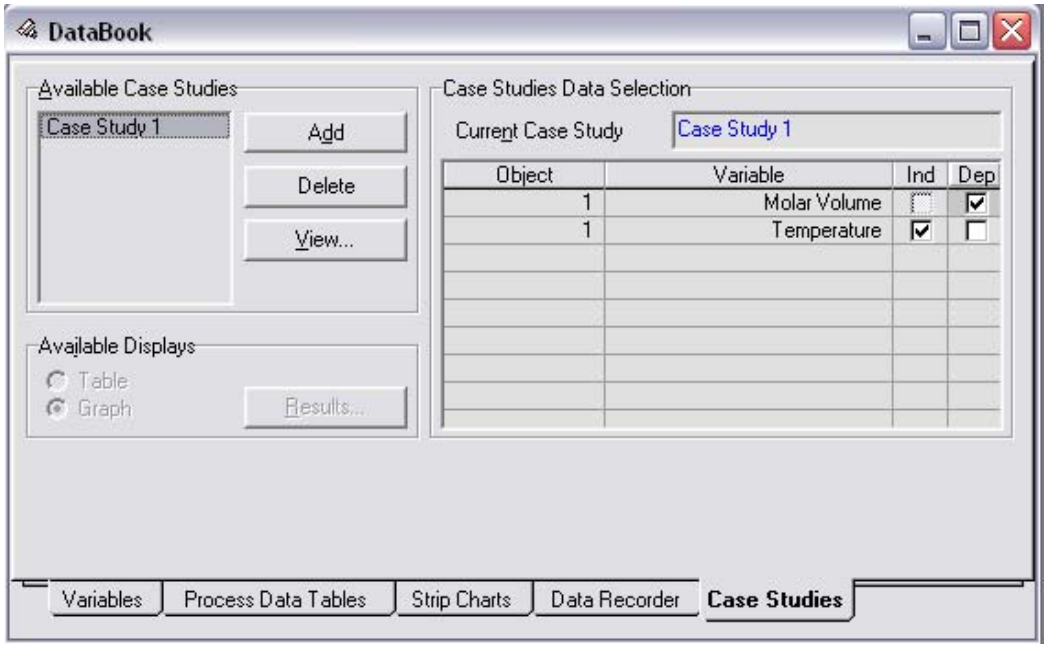


Figure 2-11

6. Click the **View** button and complete the page as shown in the Figure 2-12. (Low Bound: 450 K; High Bound: 550 K; Step Size: 10 K)

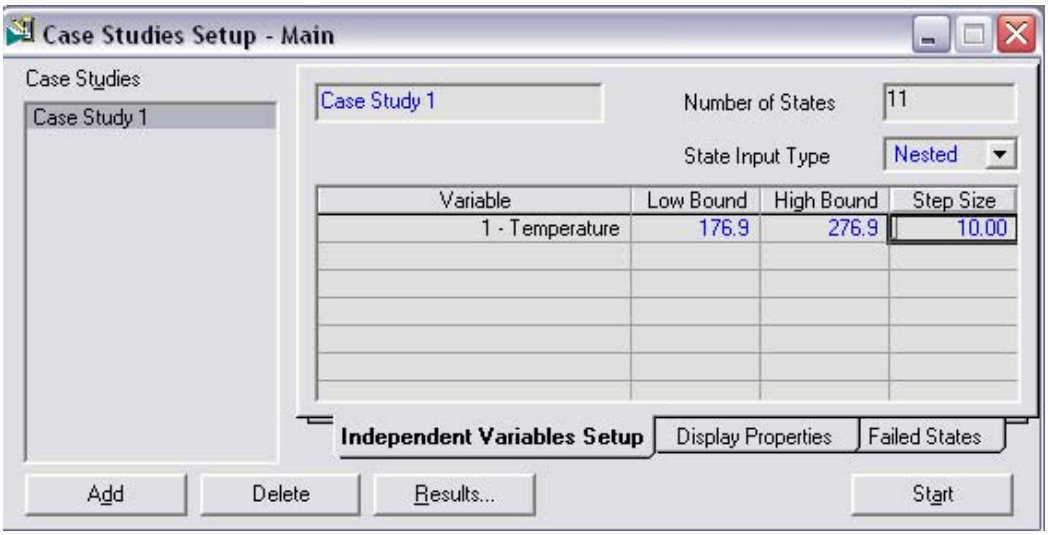


Figure 2-12

7. Click the **Start** button to start the analysis. Once the analysis finished, click **Results** to view the result.

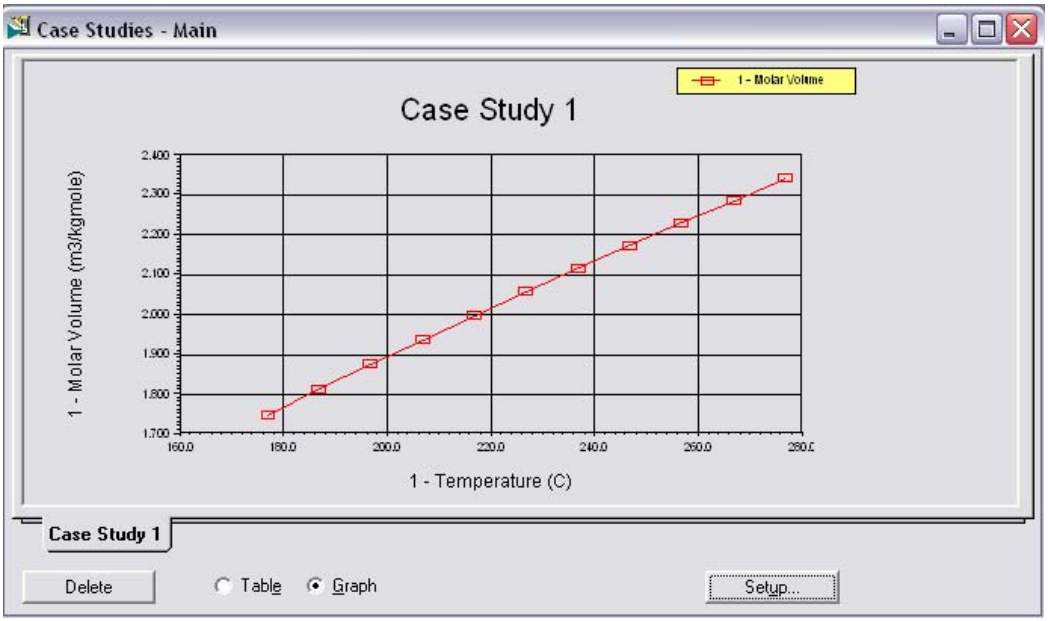


Figure 2-13

What can you conclude from this graph?

_____

_____

_____

Changing the Fluid Package

1. Press the **Enter Basis Environment** icon which is located on the menu bar.

2. This should take you to the Fluid Package window. Click on the **Prop Pkg** tab.
3. In the list in the left of the window, scroll and select **Peng Robinson** EOS.
4. Press the green arrow in the menu bar to return to the PFD.

5. Since the conditions are the same, use the saving **EOS SRK** and save it with the new name **EOS PR**.
6. Preview the result with Workbook and Case Study.

Compare the result using two different fluid packages; Soave-Redlich-Kwong and Peng-Robinson.

_____

_____

_____

2.3 Review And Summary

You have solved a very simple problem to find the specific volume of a pure component using Aspen HYSYS. When you use Aspen HYSYS, the parameters are stored in a database, and the calculations are pre-programmed. Your main concern is to use the graphical user interface (GUI) correctly.

In this chapter, you are able to preview the result using Workbook. Workbook is the most concise way to display process information in a tabular format. The Workbook is designed for this purpose and extends the concept to the entire simulation. In addition to displaying stream and general unit operation information, the Workbook is also configured to display information about any object type (streams, pipes, controllers, separators, etc.).

You are also should be to analyze the process property using Case Studies. The Case Study is used to monitor the response of key process variables to changes in your steady state process. After the Case Study solves, you can view the results in a plot.

Lastly, you are able to compare the result from two different equation of state, Peng-Robinson (PR) and Soave-Redlich-Kwong (SRK).

2.4 Problems

1. Find the molar volume of ammonia gas at 56 atm and 450 K using Soave-Redlich-Kwong (SRK) equation of state.

2. Find the molar volume of methanol gas at 100 atm and 300 ^{o}C using Peng-Robinson (PR) equation of state. Compare its molar volume when you are using Soave-Redlich-Kwong (SRK) equation of state.

3. Consider the following mixture going into a Water-Gas-Shift reactor to make hydrogen for the hydrogen economy. CO, 630 kmol/h; H_2O, 1130 kmol/h; CO_2, 189 kmol/h; H_2, 63 kmol/h. The gas is at 1 atm and 500 K. Compute the specific volume of this mixture using Soave-Redlich-Kwong (SRK) equation of state.

4. Consider a mixture of 25 percent ammonia, and the rest nitrogen and hydrogen in a 1:3 ratio. The gas is at 270 atm and 550 K. Use Peng-Robinson (PR) equation of state to compute the specific volume of this mixture.

5. Consider the following mixture that is coming out of a methanol reactor: CO, 100 kmol/h; H_2, 200 kmol/h; methanol, 100 kmol/h. The gas is at 100 atm and 300 ^{o}C. Compute the specific volume using Soave-Redlich-Kwong (SRK) equation of state and compare it with Peng-Robinson (PR) equation of state.

Chapter 3
Pump

Pump

This chapter begins with a problem to find the pump outlet temperature when given the pump efficiency. The user will operate a pump operation in HYSYS to model the pumping process. The user will learn how to connect streams to unit operations such as pump. At the end of this chapter, the user will determine the pump outlet temperature when given pump efficiency or vice versa.

The Pump operation is used to increase the pressure of an inlet liquid stream. Depending on the information specified, the Pump calculates either an unknown pressure, temperature or pump efficiency.

Learning Outcomes: At the end of this chapter, the user will be able to:

- Operate a pump operation in HYSYS to model the pumping process
- Connect streams to unit operations
- Determine the pump efficiency and outlet temperature

Prerequisites: Before beginning this chapter, the users need to know how to:

- Start HYSYS
- Select components
- Define and select a fluid package
- Add and specify material streams

3.1 Problem Statement

Pumps are used to move liquids. The pump increases the pressure of the liquid. Water at 120°C and 3 bar is fed into a pump that has only 10% efficiency. The flowrate of the water is 100 kgmole/h and its outlet pressure from the pump is 84 bar. Using Peng-Robinson equation of state as a fluid package, determine the outlet temperature of the water.

3.2 Building the Simulation

The first step in building any simulation is defining the fluid package. A brief review on how to define a fluid package and install streams is described below. *For a complete description, see Chapter 1: Starting with HYSYS.*

3.3 Accessing HYSYS

To start HYSYS:

1. Click on the **Start** menu.
2. Select **Programs | AspenTech | Aspen Engineering Suite | Aspen HYSYS 2004.1 | Aspen HYSYS 2004.1**.

Open a new case by using one of the following:

1. Go to the **File** menu, select **New**, followed by **Case**, or
2. Press **Ctrl N**, or
3. Click the **New** icon on the toolbar.

3.4 Defining the Simulation Basis

1. Enter the following values in the specified fluid package view:

On this page…	Select…
Property Package	Peng-Robinson
Components	H_2O

2. Click the **Enter Simulation Environment** button when you are ready to start building the simulation.

3.5 Installing a Stream

There are several ways to create stream:

- Press **F11**. The Stream property view appears, or
- Double-click the **Stream** icon in the **Object Palette**.

3.6 Defining Necessary Streams

Add a stream with the following values.

In this cell…	Enter…
Name	Feed
Composition	H_2O – 100%
Molar Flow	100 kgmole/h
Temperature	120°C
Pressure	3 bar

Add a second stream with the following properties.

In this cell…	Enter…
Name	Outlet
Pressure	84 bar

3.7 Adding Unit Operations

1. There are a variety of ways to add unit operations in HYSYS:

To use the…	Do this…
Menu Bar	From the **Flowsheet** menu, select **Add Operation** or Press **F12**. The **UnitOps** view appears.
Workbook	Open the **Workbook** and go to the **UnitOps** page, then click the **Add UnitOp** button. The **UnitOps** view appears.
Object Palette	From the **Flowsheet** menu, select **Open object Palette**, or press **F4**. Double-click the icon of the operation you want to add.
PFD/Object Palette	Using the right mouse button, drag ‘n’ drop the icon from the **Object Palette** to the PFD.

2. This will install a pump on the PFD as shown in Figure 3-1.

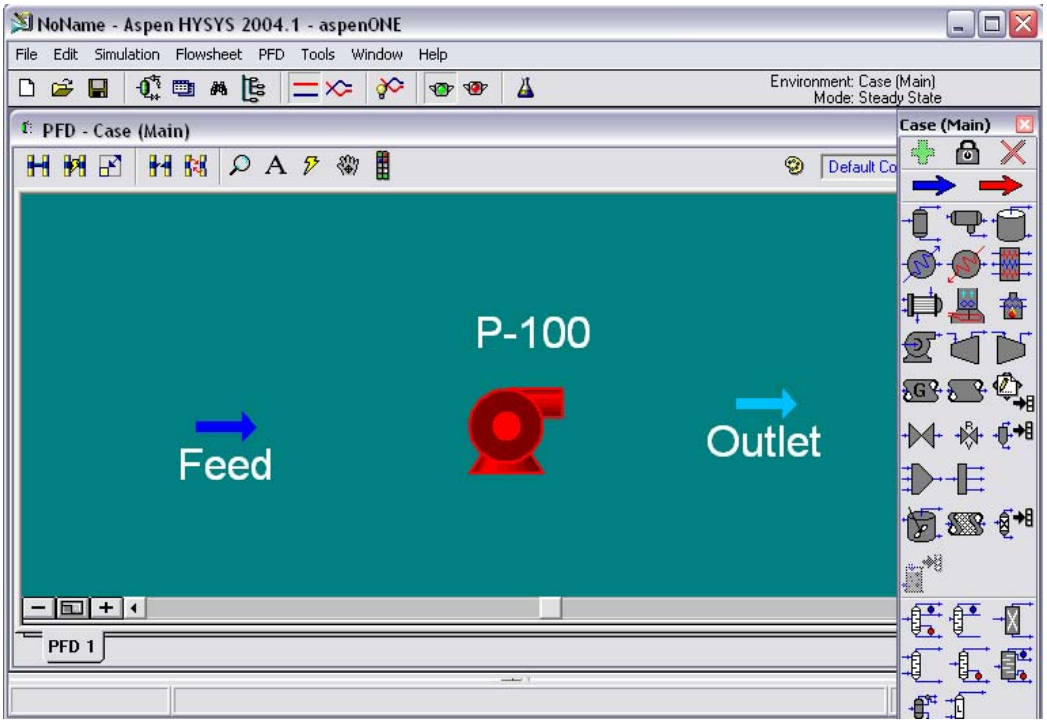


Figure 3-1: Installing Pump in HYSYS

3.8 Connecting Pump with Streams

1. From Figure 3-1, double-click on the **Pump P-100** icon to open the pump window as shown in Figure 3-2.

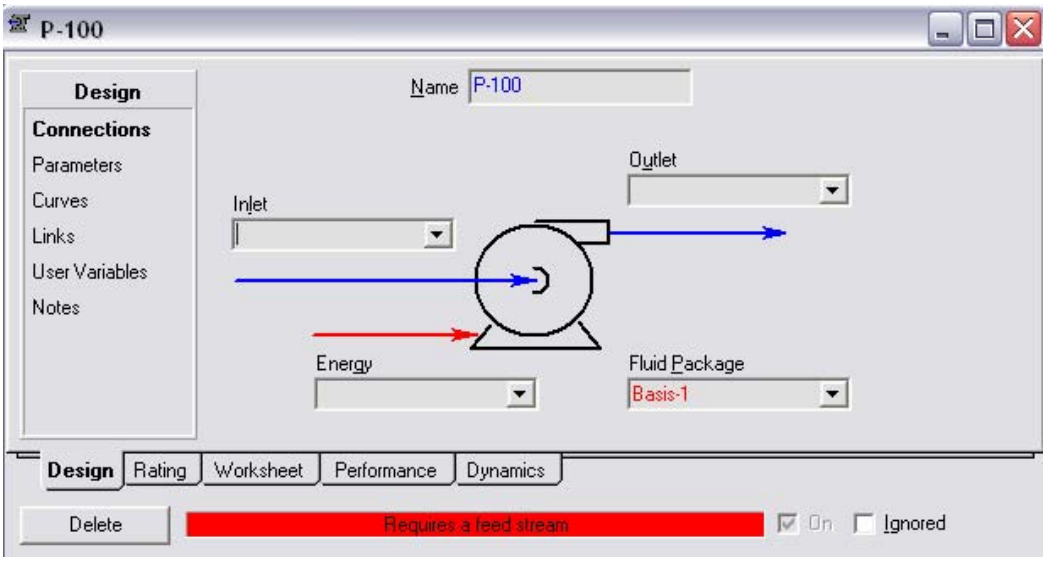


Figure 3-2: Pump Window Property

2. In the **Inlet**, scroll down to select *Feed* and *Outlet* in the **Outlet** as shown in Figure 3-3.

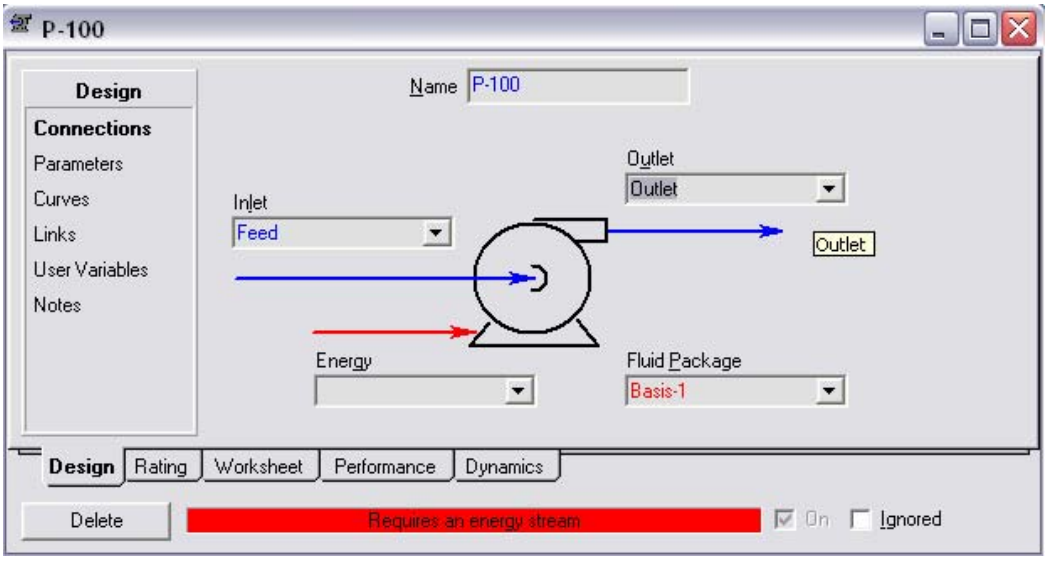


Figure 3-3: Connecting Pump with Streams

3. From Figure 3-3, the warning red message bar at the bottom of the window indicating that we need an energy stream. To create an energy stream for the pump, click to the space in the **Energy**, and type *work*. This will create energy stream name *work* for the pump as shown in Figure 3-4.

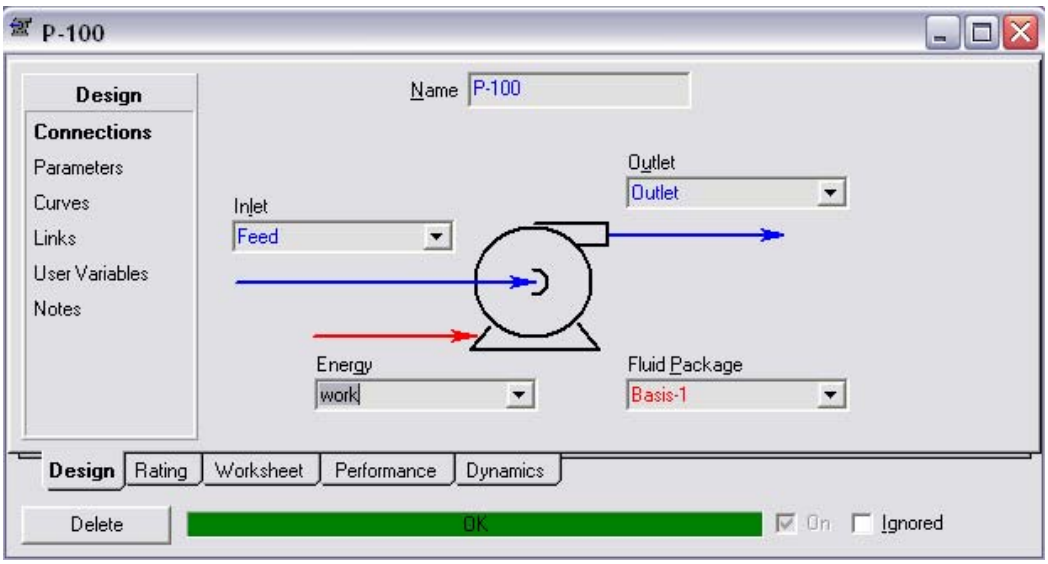


Figure 3-4: Creating Energy Stream for Pump

4. Once a pump has enough information, a green bar appears at the bottom of the window indicating that everything is "OK" (See Figure 3-4).

Tips: *For pump to have enough information, it only requires outlet pressure assuming that the inlet stream is fully specified.*

3.9 Specifying the Pump Efficiency

Default efficiency for the pump is **75%**. To change the efficiency, do the following:

1. Click on the **Design** tab of the pump window.
2. Then click on **Parameters**.
3. In the **Adiabatic Efficiency** box on the parameters page, enter **10**. The units should be in per cent as shown in Figure 3-5.

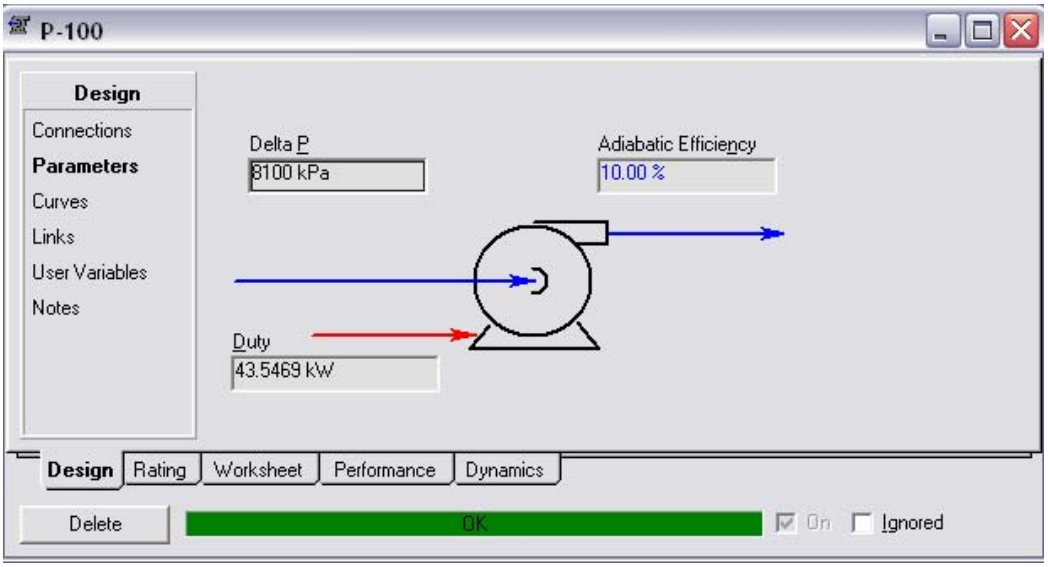


Figure 3-5: Changing Pump Efficiency

4. After the efficiency is entered the streams of the pumps should be solved. Click on the **Worksheet** tab to view the results as shown in Figure 3-6.

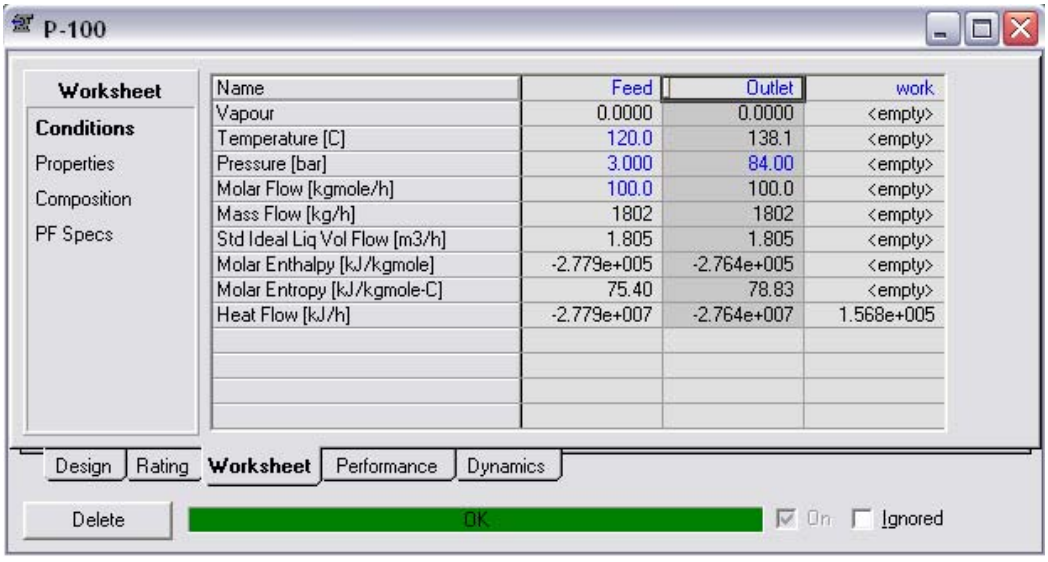


Figure 3-6: Worksheet tab in Pump

*Question: What is the outlet temperature of the water?*_____

3.10 Saving

1. Go to the **File** menu.
2. Select **Save As**.
3. Give the HYSYS file the name **Pump** then press the OK button.

3.11 Discussion

This example shows that pumping liquid can increase their temperature. In this case, the pump was only 10% efficient and it caused 18°C in the temperature of the water. The less efficient a pump is, the greater the increase in the temperature of the fluid being pumped. This arises because in a low efficient pump, more energy is needed to pump the liquid to get the same outlet pressure of a more efficient pump. So the extra energy gets transferred to the fluid.

3.12 Review and Summary

In the first part of this chapter, we started with a problem to find the pump outlet temperature when given the pump efficiency. Pump basically used to move liquids. In this chapter the user operated a pump operation in HYSYS to model the pumping process. The user also been trained on how to connect streams to unit operations such as pump.

At the end of this chapter, the user was trained to determine the pump outlet temperature when the pump efficiency was given. On the other hand, when the outlet temperature was given, the pump efficiency can be determined using HYSYS.

3.13 Further Study

If the outlet temperature is 200^{o}C, what is the efficiency of the pump?

Chapter 4
Compressor

Compressor

This chapter begins with a problem to find the compressor outlet temperature when given the compressor efficiency. The user will operate a compressor operation in HYSYS to model the compressing process. At the end of this chapter, the user will determine the compressor outlet temperature when given compressor efficiency or vice versa.

The Compressor operation is used to increase the pressure of an inlet gas stream. Depending on the information specified, the Compressor calculates ether a stream property (pressure or temperature) or compression efficiency.

Learning Outcomes: At the end of this chapter, the user will be able to:

- Define a new component using hypotheticals
- Operate a compressor operation in HYSYS to model the compressing process
- Determine the compressor efficiency and outlet temperature

Prerequisites: Before beginning this chapter, the users need to know how to:

- Start HYSYS
- Select components
- Define and select a fluid package
- Add and specify material streams

4.1 Problem Statement

Compressors are used to move gases. The compressor increases the pressure of the gases. A mixture of natural gas (C_1, C_2, C_3, i-C_4, n-C_4, i-C_5, n-C_5, n-C_6, C_7^+) at 100°C and 1 bar is fed into a compressor that has only 30% efficiency. The flowrate of the natural gas is 100 kgmole/h and its outlet pressure from the compressor is 5 bar. Using Peng-Robinson equation of state as a fluid package, determine the outlet temperature of the natural gas.

4.2 Accessing HYSYS

To start HYSYS:

1. Click on the **Start** menu.
2. Select **Programs | AspenTech | Aspen Engineering Suite | Aspen HYSYS 2004.1 | Aspen HYSYS 2004.1**.

Open a new case by using one of the following:

1. Go to the **File** menu, select **New**, followed by **Case**, or
2. Press **Ctrl N**, or
3. Click the **New** icon on the toolbar.

4.3 Defining the Simulation Basis

1. Enter the following values in the specified fluid package view:

On this page…	Select…
Property Package	Peng-Robinson
Components	C_1, C_2, C_3, i-C_4, n-C_4, i-C_5, n-C_5, n-C_6, C_7^+

2. Component C_7^+ is not available in the Component Library. Therefore, you need to create this component using **Hypothetical.**

4.4 Defining a New Component

1. Click the **Hypothetical** menu item in the **Add Component** box to add a hypothetical component to the Fluid Package

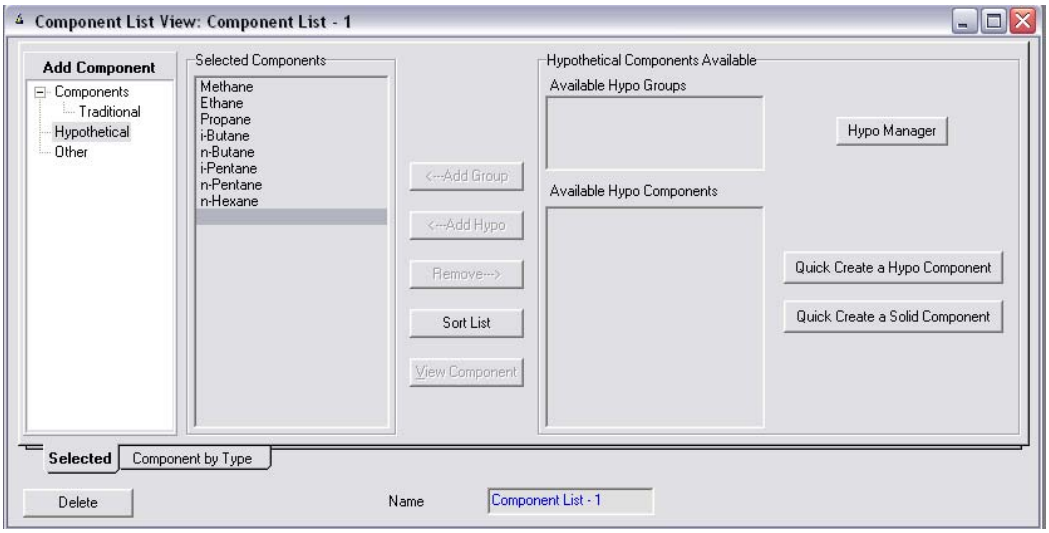


Figure 4-1

2. Click **Quick Create a Hypo Component** to create a hypothetical component.

A hypothetical component can be used to model non-library components, defined mixtures, undefined mixtures, or solids. You will be using a hypothetical component to model the component in the gas mixture heavier than hexane.

3. In the view for the hypo component you are creating, click the **ID** tab and in the **Component Name** cell type **C7+**.

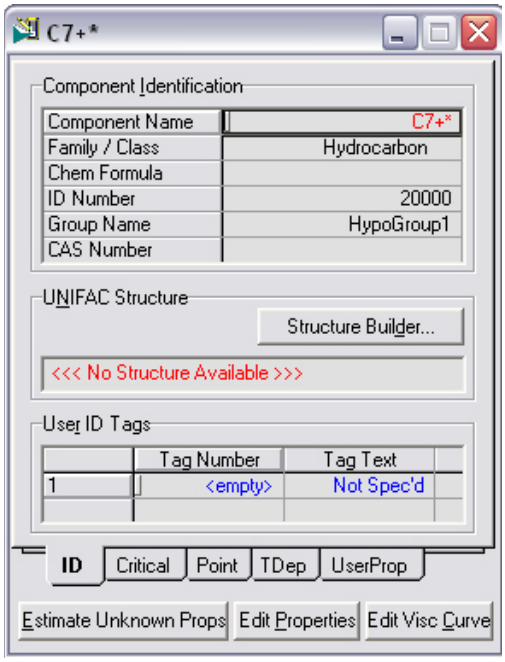


Figure 4-2

Since you do not know the structure of the hypothetical component and you are modeling a mixture, the Structure Builder will not be used.

4. Select the **Critical** tab. The only property supplied by the lab for the C7+ component is the **Normal Boiling Pt**. Enter a value of **110°C** (**230°F**).
5. Click Estimate Unknown Props to estimate all the other properties and fully define the hypothetical component.

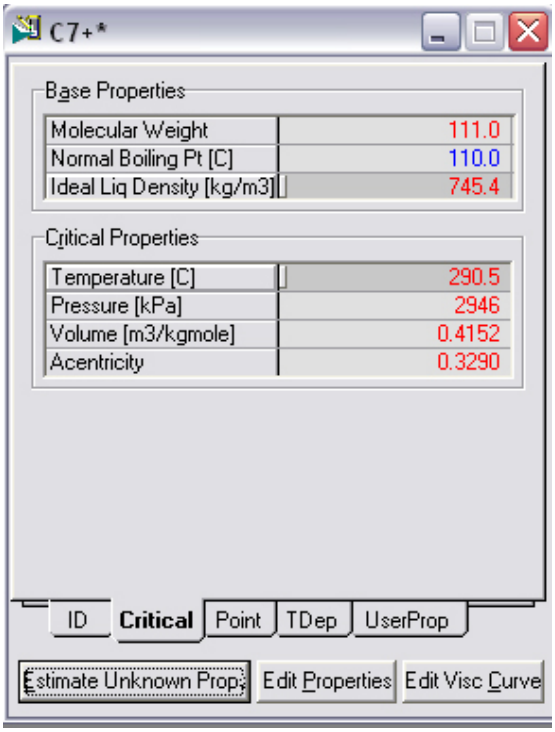


Figure 4-3

The minimum information required for defining a hypo is the Normal Boiling Pt or the Molecular Weight and Ideal Liq Density.

6. When the hypo component has been defined, return to the fluid package by closing the hypo component C7+* view.
7. Add the hypo component to the **Selected Components** list by selecting it in the **Available Hypo Components** list and then clicking the **Add Hypo** button.

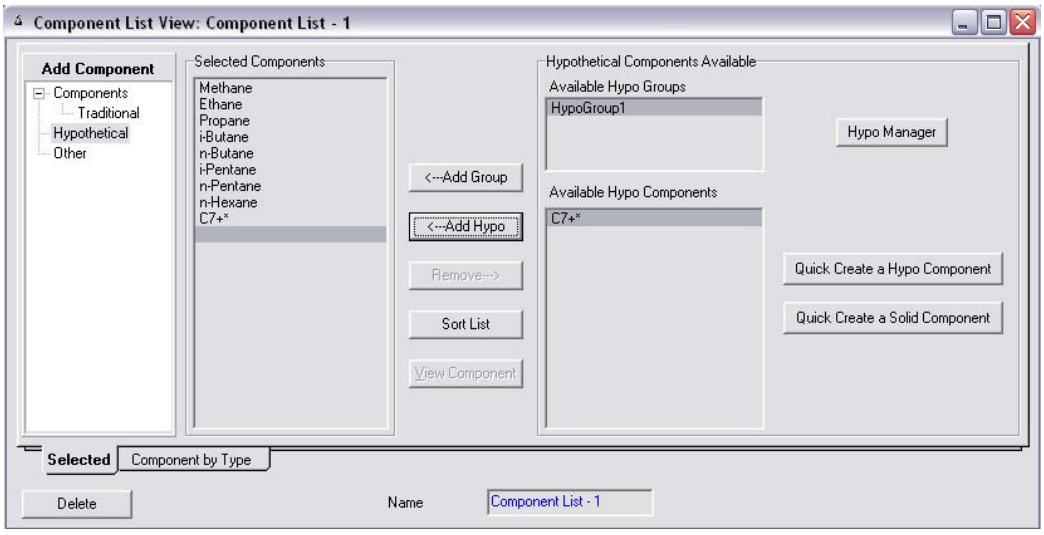


Figure 4-4

Every hypo you create is part of a Hypo Group. By default, this hypo is placed in **HypoGroup1**. You can add additional groups and move hypo components between groups. This is done on the **Hypotheticals** tab of the **Simulation Basis Manager**.

Compare the properties of C7+ with C7 and C8			
	C7+	**C7**	**C8**
Normal Boiling Point			
Ideal Liquid Density			
Molecular Weight			

You will need to add components C7 and C8 to the component list in order to view their properties. Ensure that you delete them once this exercise is finished.

8. You have now finished defining the fluid package. Click the **Enter Simulation Environment** button when you are ready to start building the simulation.

4.5 Installing a Stream

There are several ways to create stream:

- Press **F11**. The Stream property view appears, or
- Double-click the **Stream** icon in the **Object Palette**.

4.6 Adding a Feed Stream

Add a new **Material** stream with the following values.

In this cell…	Enter…
Name	Natural Gas
Temperature	100°C
Pressure	1 bar
Molar Flow	100 kgmole/h
Component Mole Fraction	
C_1	0.330
C_2	0.143
C_3	0.101
i-C_4	0.098
n-C_4	0.080
i-C_5	0.069
n-C_5	0.059
n-C_6	0.078
C_7^+	0.042

4.7 Adding a Compressor

1. There are several ways to add unit operations. For a complete description, see **Chapter 3** (**Adding Unit Operations**).

   - Press the **F12** hot key. Select the desired unit operation from the Available Unit operations group.
   - Double-click on the unit operation button in the **Object Palette**.

2. On the **Connections** tab, add a Compressor and enter the following information as shown in Figure 4-1:

In this cell…	Enter…
Name	Compressor
Feed	Natural Gas
Outlet	Comp_Out
Energy	Work

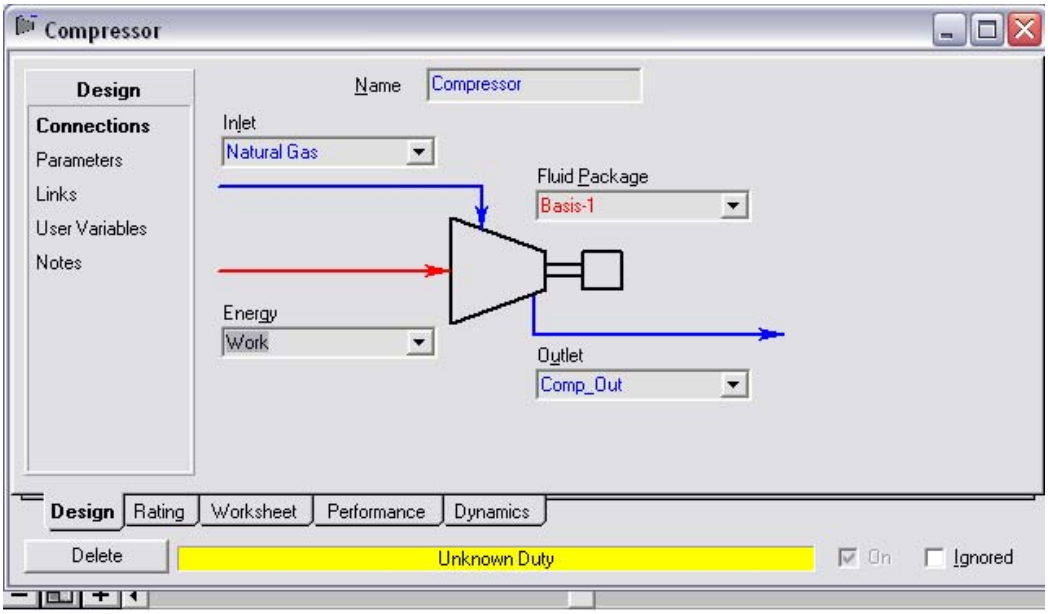


Figure 4-5

3. Switch to the **Parameters** page. Change the Adiabatic Efficiency to **30%**.

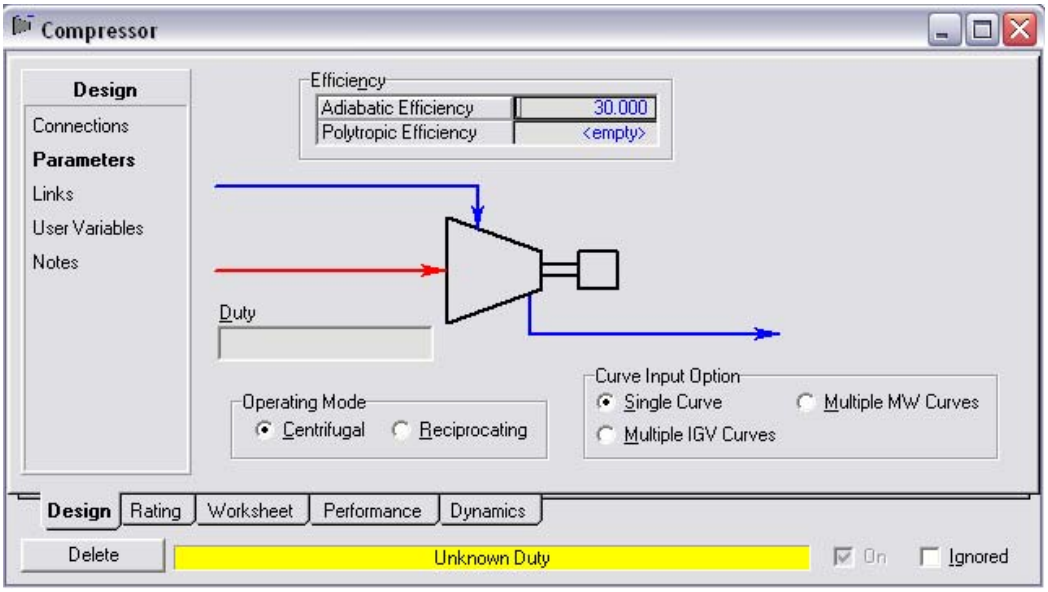


Figure 4-6

4. Go to the **Worksheet** tab. On the **Conditions** page, complete the page as shown in the following figure. The pressure for Comp_Out will be **5** bar.

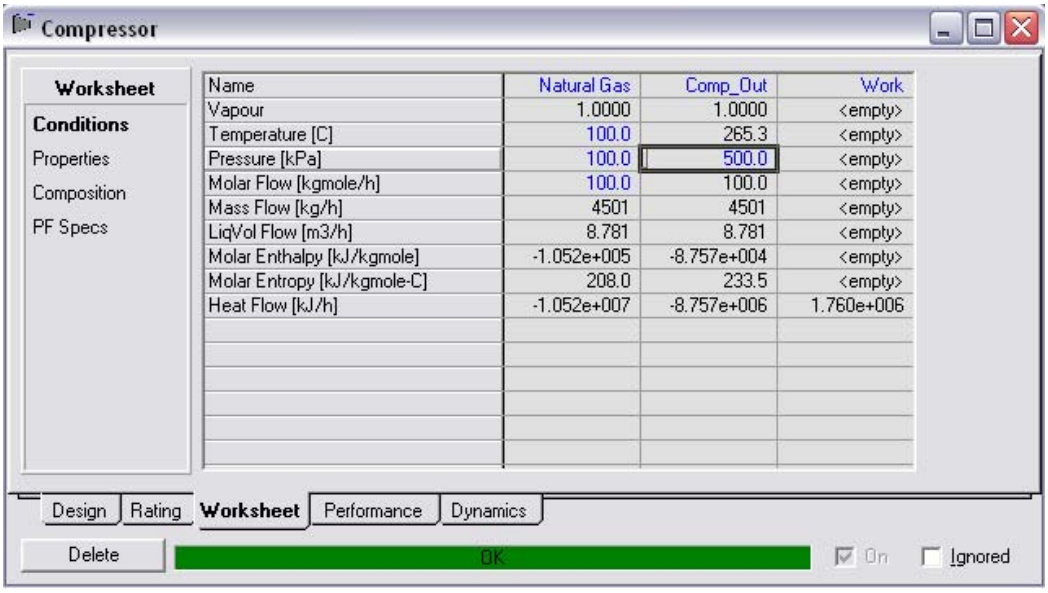


Figure 4-7

What is the outlet temperature of the compressor? _____

4.8 Save Your Case

1. Go to the **File** menu.
2. Select **Save As**.
3. Give the HYSYS file the name **Compressor** then press the OK button.

4.9 Discussion

This example shows that compressing gases can increase their temperature. In this case, the compressor was only 30% efficient and it caused 165.3°C increase in the temperature of the natural gas. The less efficient a compressor is, the greater the increase in the temperature of the gases being compressed.

4.10 Review and Summary

In the first part of this chapter, we started with a problem to find the compressor outlet temperature when given the compressor efficiency. Compressor basically used to move gases. In this chapter the user operated a compressor operation in HYSYS to model the compressing process.

At the end of this chapter, the user was trained to determine the compressor outlet temperature when the compressor efficiency was given.

4.11 Further Study

If the outlet temperature is 400^{o}C, what is the efficiency of the compressor?

Chapter 5
Expander

Expander

This chapter begins with a problem to find the expander outlet temperature when given the expander efficiency. The user will operate an expander operation in HYSYS to model the expansion process. At the end of this chapter, the user will determine the expander outlet temperature when given expansion efficiency or vice versa.

The Expander operation is used to decrease the pressure of a high pressure inlet gas stream to produce an outlet stream with low pressure and high velocity. An expansion process involves converting the internal energy of the gas to kinetic energy and finally to shaft work. The Expander calculates either a stream property or an expansion efficiency.

There are several methods for the Expander to solve, depending on what information has been specified. In general, the solution is a function of flow, pressure change, applied energy, and efficiency. The Expander provides a great deal of flexibility with respect to what you can specify and what it then calculates. You must ensure that you do not enable too many of the solution options or inconsistencies may result.

Learning Outcomes: At the end of this chapter, the user will be able to:

- Operate an expander operation in HYSYS to model the expansion process
- Determine the expansion efficiency and outlet temperature

Prerequisites: Before beginning this chapter, the users need to know how to:

- Start HYSYS
- Select components
- Define and select a fluid package
- Add and specify material streams

5.1 Problem Statement

The Expander operation is used to decrease the pressure of a high pressure inlet gas stream to produce an outlet stream with low pressure and high velocity. A mixture of natural gas (methane, ethane and propane) at 25°C and 20 bar is fed into an expander that has only 30% efficiency. The flowrate of the natural gas is 100 kgmole/h and its outlet pressure from the compressor is 5 bar. Using Peng-Robinson equation of state as a fluid package, determine the outlet temperature of the natural gas.

5.2 Defining the Simulation Basis

1. Enter the following values in the specified fluid package view:

On this page…	Select…
Property Package	Peng-Robinson
Components	C_1, C_2, C_3

2. Click the **Enter Simulation Environment** button when you are ready to start building the simulation.

5.3 Adding a Feed Stream

Add a new **Material** stream with the following values.

In this cell…	Enter…
Name	Natural Gas
Temperature	25°C
Pressure	20 bar
Molar Flow	100 kgmole/h
Component Mole Fraction	
C_1	0.500
C_2	0.300
C_3	0.200

5.4 Adding an Expander

1. Double-click on the **Expander** button on the **Object Palette**.
2. On the **Connections** page, enter the following information:

In this cell…	Enter…
Name	Expander
Feed	Natural Gas
Outlet	Out
Energy	Work

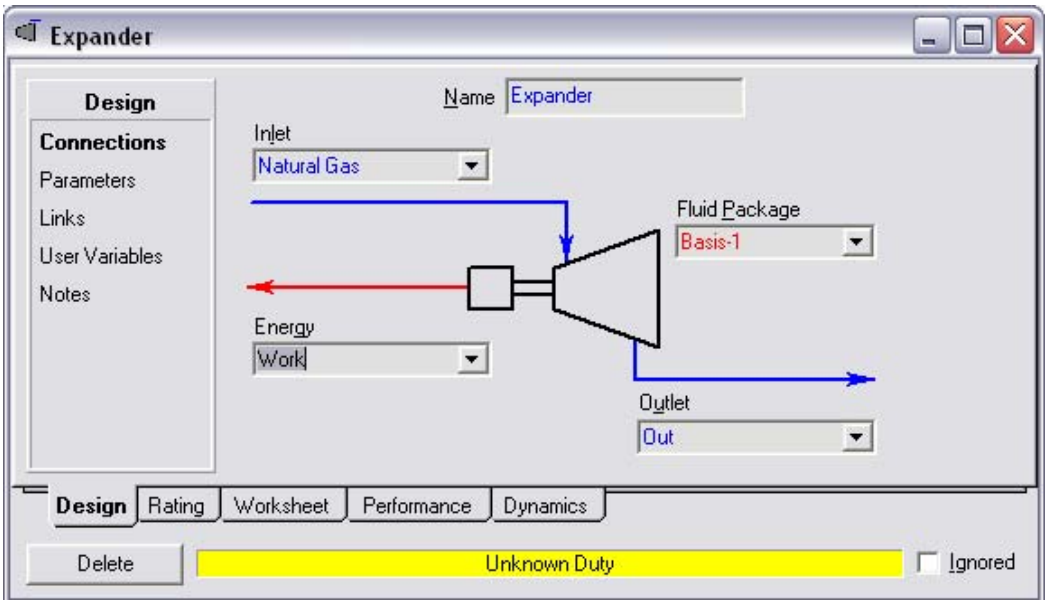


Figure 5-1

3. Switch to the **Parameters** page. Change the Adiabatic Efficiency to **30%**.

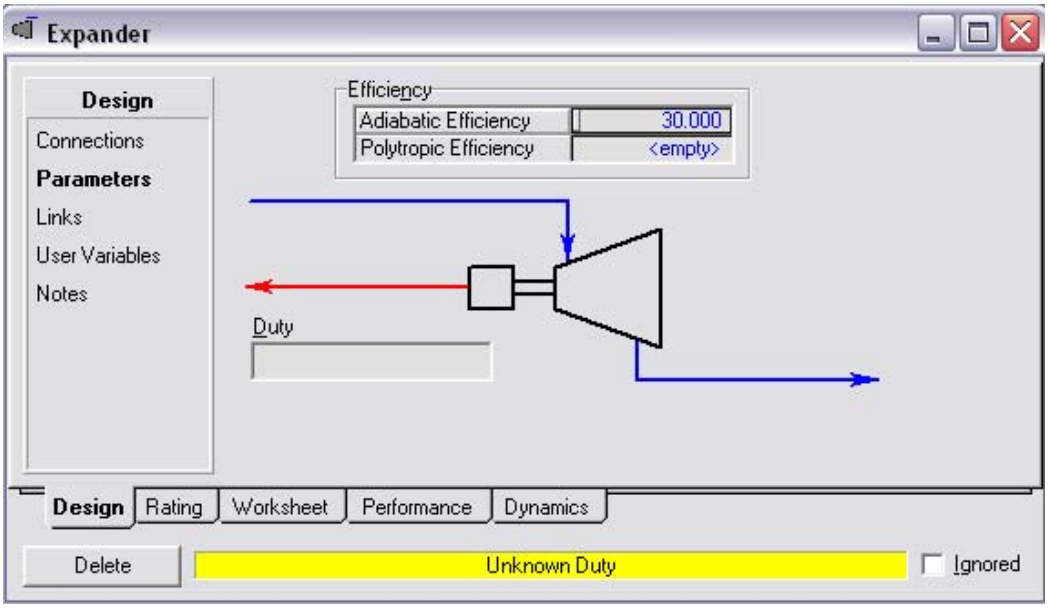


Figure 5-2

4. Go to the **Worksheet** tab. On the **Conditions** page, complete the page as shown in the following figure. The pressure for Out will be **5** bar.

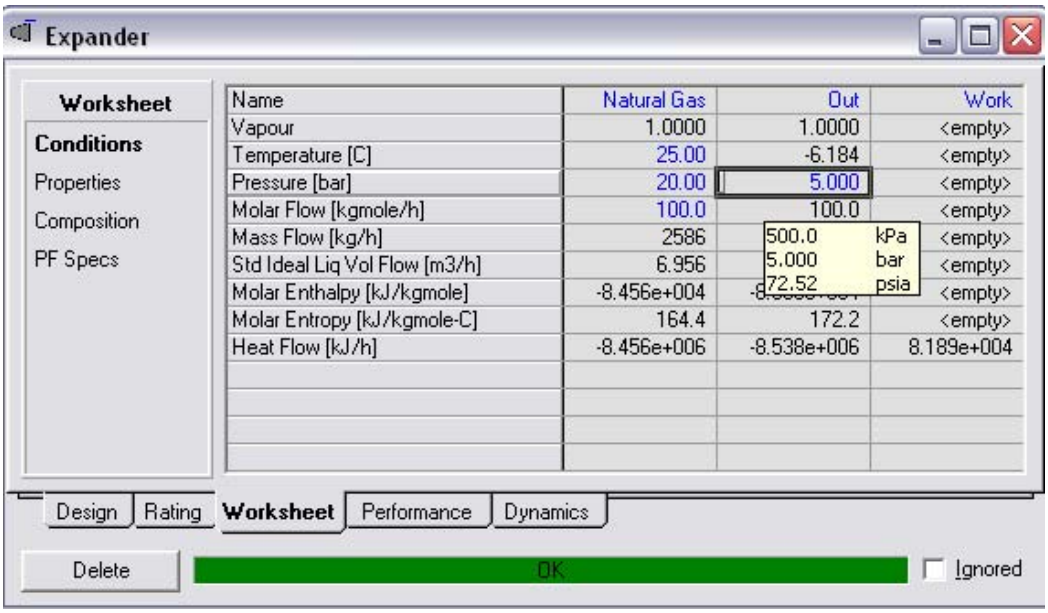


Figure 5-3

What is the outlet temperature of the expander? _____

5.5 Save Your Case

1. Go to the **File** menu.
2. Select **Save As**.
3. Give the HYSYS file the name **Expander** then press the OK button.

5.6 Discussion

This example shows that expansion gases can decrease their temperature. In this case, the expander was only 30% efficient and it caused 31°C decrease in the temperature of the natural gas. The less efficient a compressor is, the less the decrease in the temperature of the gases being expanded.

5.7 Review and Summary

In the first part of this chapter, we started with a problem to find the expander outlet temperature when given the expansion efficiency. The Expander operation is used to decrease the pressure of a high pressure inlet gas stream to produce an outlet stream with low pressure and high velocity. In this chapter the user operated an expander operation in HYSYS to model the expansion process.

At the end of this chapter, the user was trained to determine the expander outlet temperature when the expansion efficiency was given.

5.8 Further Study

If the outlet temperature is -30^{o}C, what is the efficiency of the expander?

Chapter 6
Heat Exchanger

Heat Exchanger

This chapter begins with a problem to find the flowrate of the cold stream passing through the heat exchanger at the given stream conditions. In this chapter, HYSYS's shell and tube heat exchanger will be used to model the process. The heat exchanger performs two-sided energy and material balance calculations. The heat exchanger is very flexible, and can solve for temperatures, pressures, heat flows (including heat loss and heat leak), material streams flows, or UA.

In HYSYS, you can choose the Heat Exchanger Model for your analysis. Your choices include an End Point analysis design model, an ideal (Ft=1) counter-current Weighted designed model, a steady state rating method, and a dynamic rating method for use in dynamic simulations. The dynamic rating method is available as either a Basic or Detailed model, and can also be used in Steady State mode for Heat Exchanger rating.

Learning Outcomes: At the end of this chapter, the user will be able to:

- Operate a heat exchanger operation in HYSYS to model the heat transfer process

Prerequisites: Before beginning this chapter, the users need to know how to:

- Start HYSYS
- Select components
- Define and select a fluid package
- Add and specify material streams

6.1 Problem Statement

Hot water at 250°C and 1000 psig is used to heat a cold stream of water in a shell and tube heat exchanger. The inlet temperature and pressure of the cold stream is 25°C and 130 psig, respectively. The outlet temperatures of the cold and hot streams are 150°C and 190°C, respectively. If the flow rate of the hot stream is 100 kg/h, determine the flow rate of the cold stream passing through the exchanger.

6.2 Solution Outline

1. Use HYSYS' shell and tube heat exchanger to model the process.
2. Define the inlet and outlet conditions for the streams as given in the problem statement.
3. Obtain the mass flowrate of the cold stream.

6.3 Building the Simulation

1. Defining components list and fluid package
2. Adding streams and unit operation

6.4 Defining the Simulation Basis

1. Enter the following values in the specified fluid package view:

On this page…	Select…
Property Package	Peng-Robinson
Components	H_2O

2. Click the **Enter Simulation Environment** button when you are ready to start building the simulation.

6.5 Adding a Feed Stream

Add a new **Material** stream with the following values.

In this cell…	Enter…
Name	Tube in
Temperature	250°C
Pressure	1000 psig
Mass Flow	100 kg/h
Compositions	H_2O – 100%

Add another new **Material** stream with the following values.

In this cell…	Enter…
Name	Shell in
Temperature	25°C
Pressure	130 psig
Compositions	H_2O – 100%

6.6 Adding a Heat Exchanger

The heat exchanger performs two-sided energy and material balance calculations. The heat exchanger is capable of solving the temperatures, pressures, heat flows (including heat loss and heat leak), material stream flows, and UA.

1. Double-click on the **Heat Exchanger** button on the **Object Palette**.
2. On the **Connections** page, enter the following information:

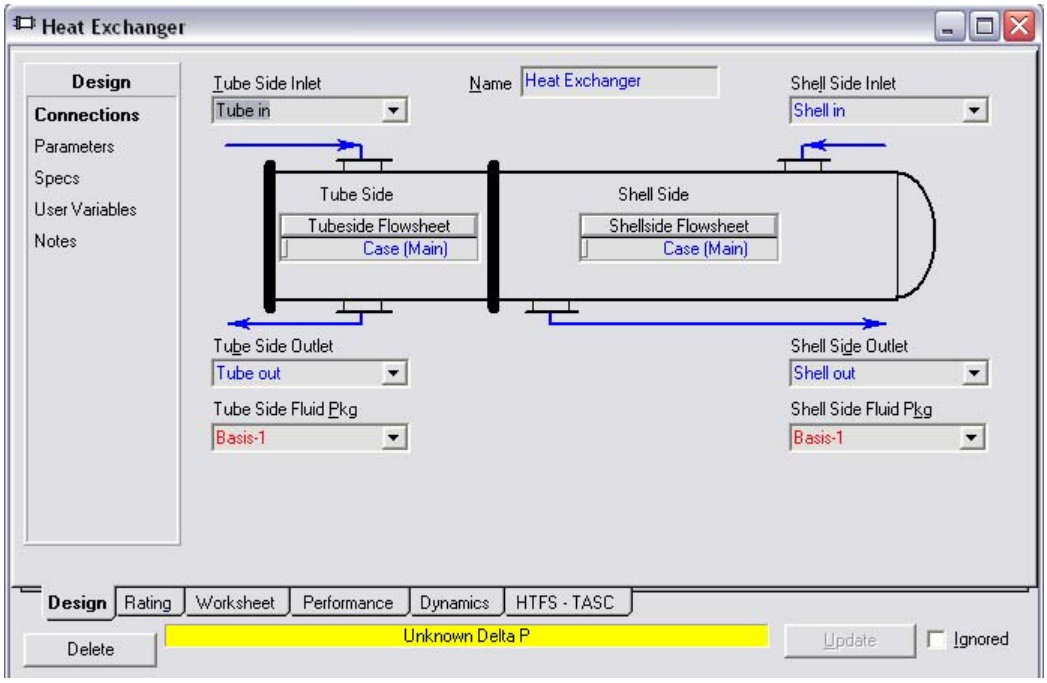


Figure 6-1

3. Switch to the **Parameters** page. Complete the page as shown in the Figure 6-2. The pressure drops for the Tube and Shell sides, will be 0 kPa.

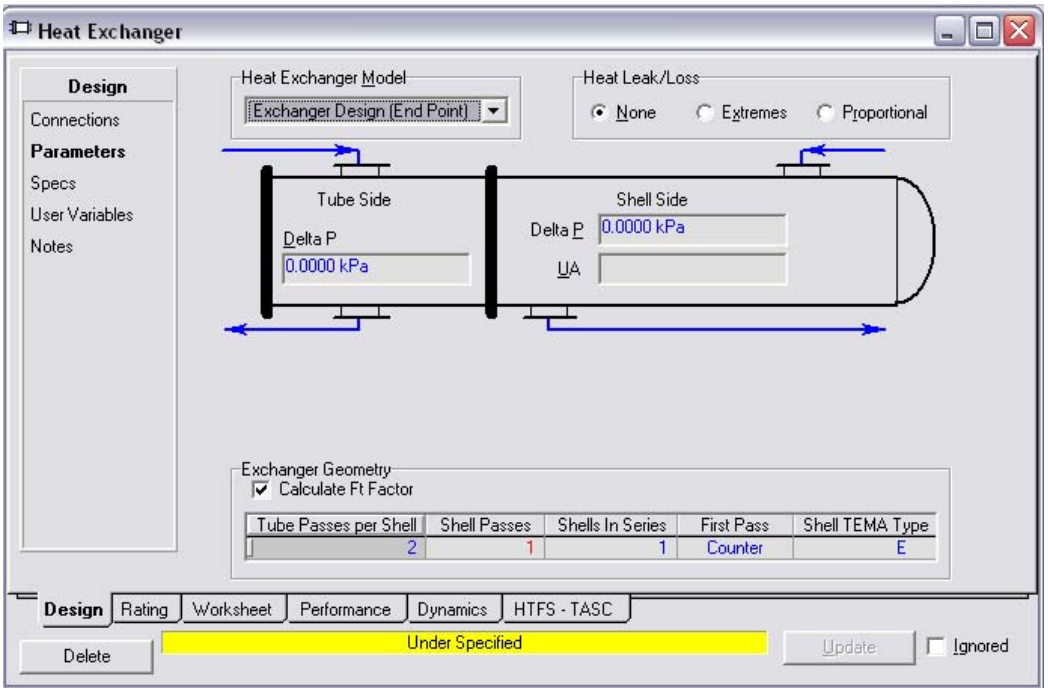


Figure 6-2

4. Go to the **Worksheet** tab. On the **Conditions** page, complete the page as shown in the following figure. The temperature for Shell out and Tube out will be 150°C and 190°C, respectively.

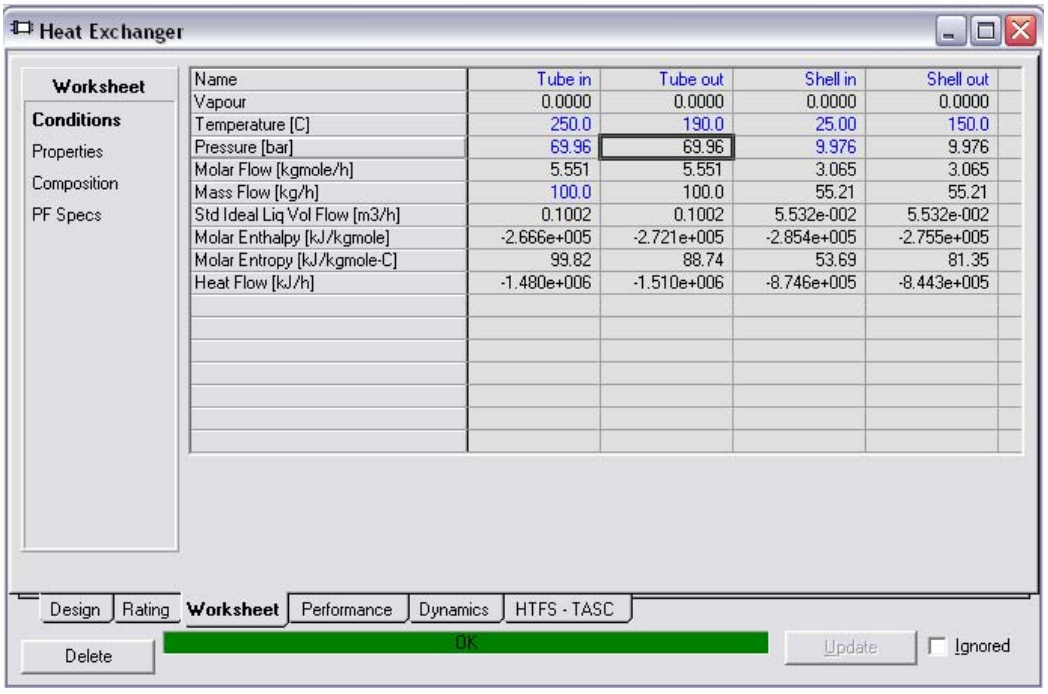


Figure 6-3

What is the mass flowrate of the cold stream? _____

6.7 Save Your Case

1. Go to the **File** menu.
2. Select **Save As**.
3. Give the HYSYS file the name **Heat Exchanger** then press the OK button.

6.8 Discussion

At the given stream conditions and a hot stream floweate of 100 kg/h, the flowrate of the cold stream passing through the heat exchanger is approximately 55.21 kg/h.

6.9 Review and Summary

In this chapter, the user was asked to find the flowrate of the cold stream passing through the heat exchanger at the given stream conditions. To me the process, HYSYS's shell and tube heat exchanger was used.

6.10 Further Study

If the flow rate of the cold stream is 100 kg/h, determine the flow rate of the hot stream passing through the exchanger. What is amount of heat transferred from the hot stream to the cold stream?

Chapter 7
Flash Separator

Flash Separator

This chapter begins with a problem to find the flowrate of the liquid and vapor outlet streams of the flash separator. In steady state mode, the Separator divides the vessel contents into its constituent vapor and liquid phases. The vapor and liquid in the vessel are allowed to reach equilibrium, before they are separated.

A Flash Separator is performed to determine the product conditions and phases. The pressure at which the flash is performed is the lowest feed pressure minus the pressure drop across the vessel. The enthalpy is the combined feed enthalpy plus or minus the duty.

The Separator has the ability to back-calculate results. In addition to the standard application (completely defined feed stream(s) being separated at the vessel pressure and enthalpy), the Separator can also use a known product composition to determine the composition(s) of the other product stream(s), and by a balance the feed composition.

Learning Outcomes: At the end of this chapter, the user will be able to:

- Operate a flash separator operation in HYSYS to model the flash separation process

Prerequisites: Before beginning this chapter, the users need to know how to:

- Start HYSYS
- Select components
- Define and select a fluid package
- Add and specify material streams

7.1 Problem Statement

We have a stream containing 15% ethane, 20% propane, 60% i-butane and 5% n-butane at 50°F and atmospheric pressure, and a flowrate of 100 lbmole/hr. This stream is to be compressed to 50 psia, and then cooled to 32°F. The resulting vapour and liquid are to be separated as the two product streams. What are the flowrates and compositions of these two streams?

7.2 Defining the Simulation Basis

1. Enter the following values in the specified fluid package view:

On this page…	Select…
Property Package	Peng-Robinson
Components	Ethane, propane, i-butane, n-butane

2. Click the **Enter Simulation Environment** button when you are ready to start building the simulation.

7.3 Adding a Feed Stream

Add a new **Material** stream with the following values.

In this cell…	Enter…
Name	Gas
Temperature	50°F
Pressure	1 atm
Molar Flow	100 lbmole/hr
Compositions	ethane – 15%
	propane – 20%
	i-butane – 60%
	n-butane – 5%

7.4 Adding a Compressor

1. Double-click on the **Compressor** button on the **Object Palette**.
2. On the **Connections** page, enter the following information:

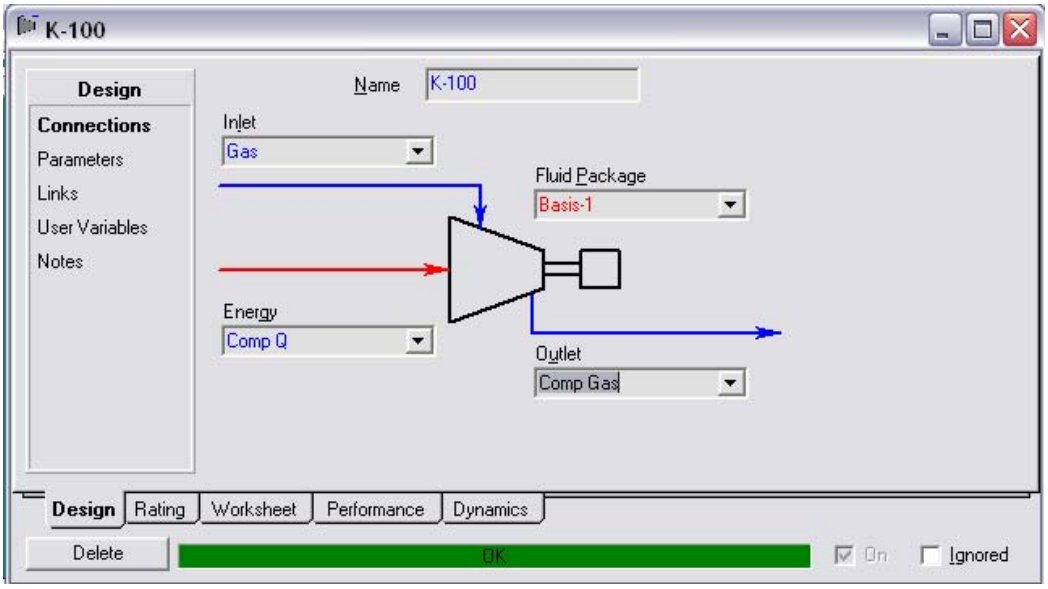
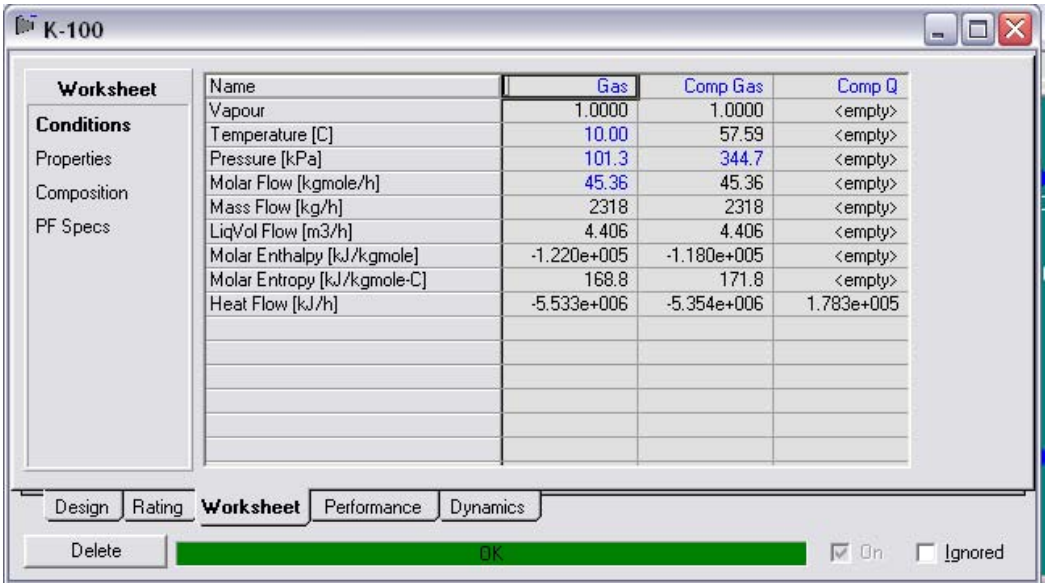


Figure 7-1

3. Go to the **Worksheet** tab. At the **Conditions** page, complete the page as shown in the Figure 7-2. The pressure for the Comp Gas is 50 psia.



Name	Gas	Comp Gas	Comp Q
Vapour	1.0000	1.0000	<empty>
Temperature [C]	10.00	57.59	<empty>
Pressure [kPa]	101.3	344.7	<empty>
Molar Flow [kgmole/h]	45.36	45.36	<empty>
Mass Flow [kg/h]	2318	2318	<empty>
LiqVol Flow [m3/h]	4.406	4.406	<empty>
Molar Enthalpy [kJ/kgmole]	-1.220e+005	-1.180e+005	<empty>
Molar Entropy [kJ/kgmole-C]	168.8	171.8	<empty>
Heat Flow [kJ/h]	-5.533e+006	-5.354e+006	1.783e+005

Figure 7-2

7.5 Adding a Cooler

1. Double-click on the **Cooler** button on the **Object Palette**.
2. On the **Connections** page, enter the following information:

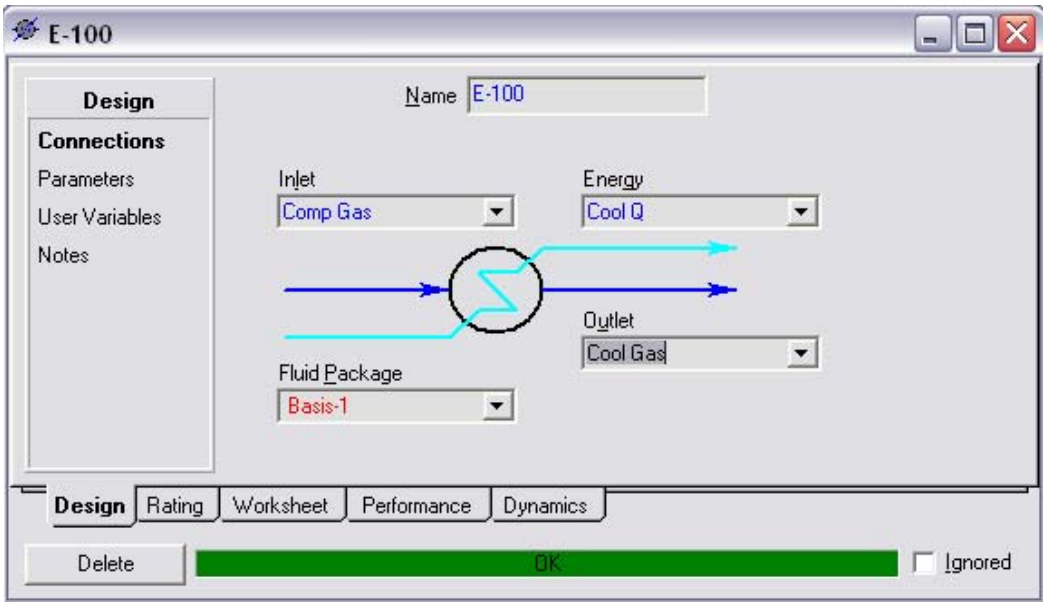


Figure 7-3

3. Switch to the **Parameters** page and complete the page as shown in the Figure 7-4. The pressure drop is 0 psia.

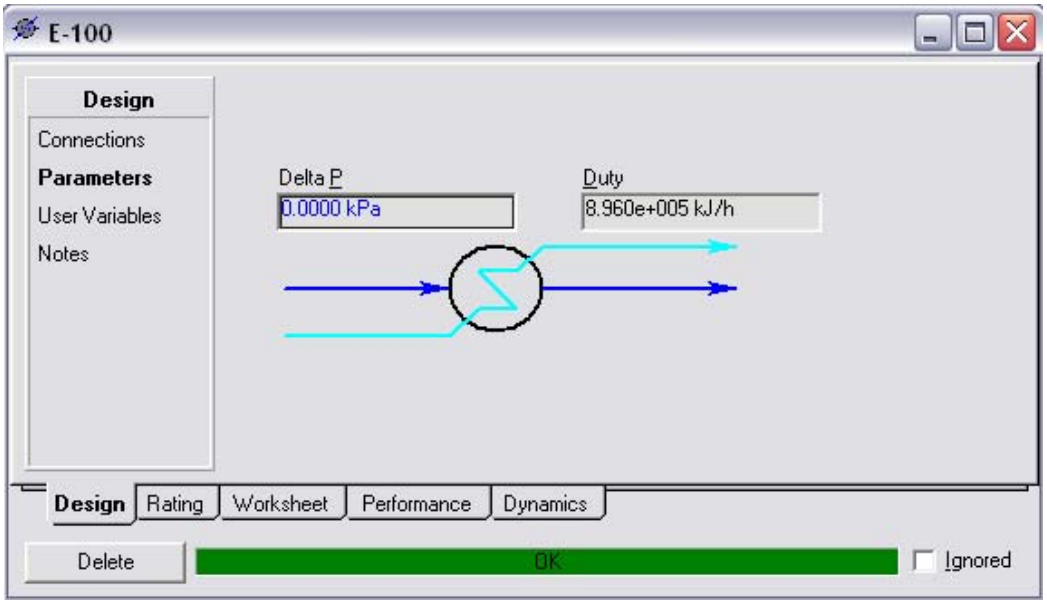


Figure 7-4

4. Go to the **Worksheet** tab. At the **Conditions** page, complete the page as shown in the Figure 7-5. The temperature for the Cool Gas is 32°F.

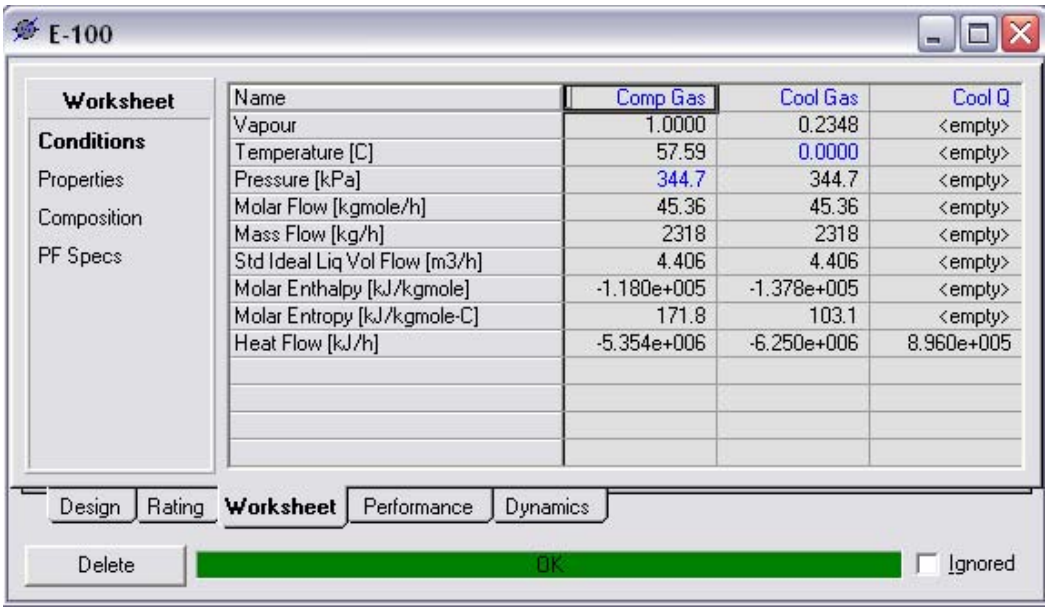


Figure 7-5

7.6 Adding a Flash Separator

1. Double-click on the **Separator** button on the **Object Palette**.
2. On the **Connections** page, enter the following information:

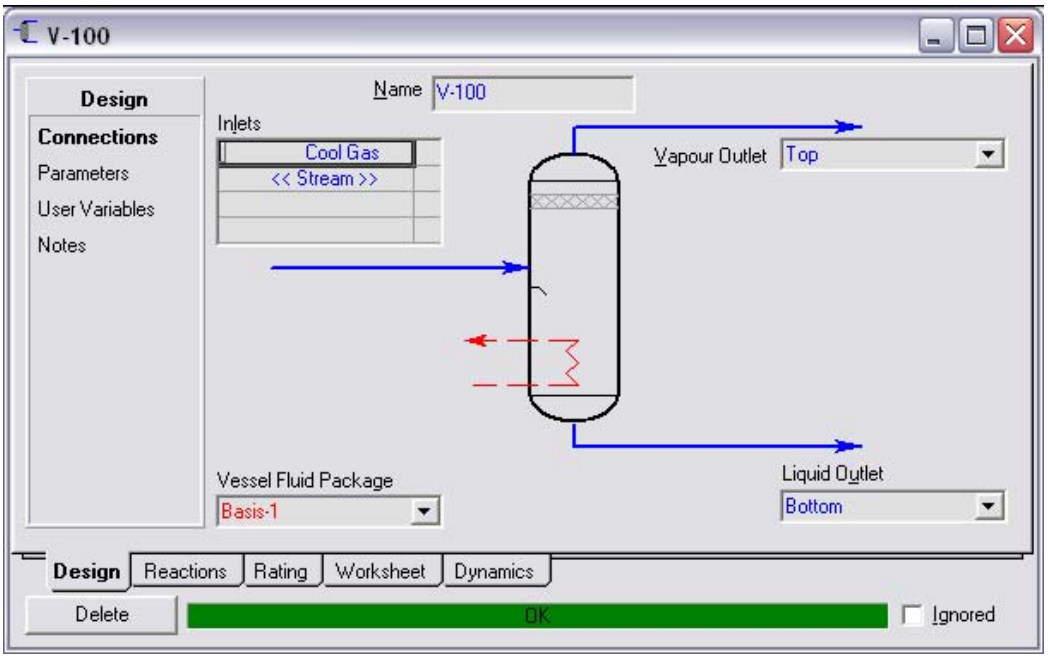


Figure 7-6

3. Go to the **Worksheet** tab to preview the result as shown in the Figure 7-7 and Figure 7-8.

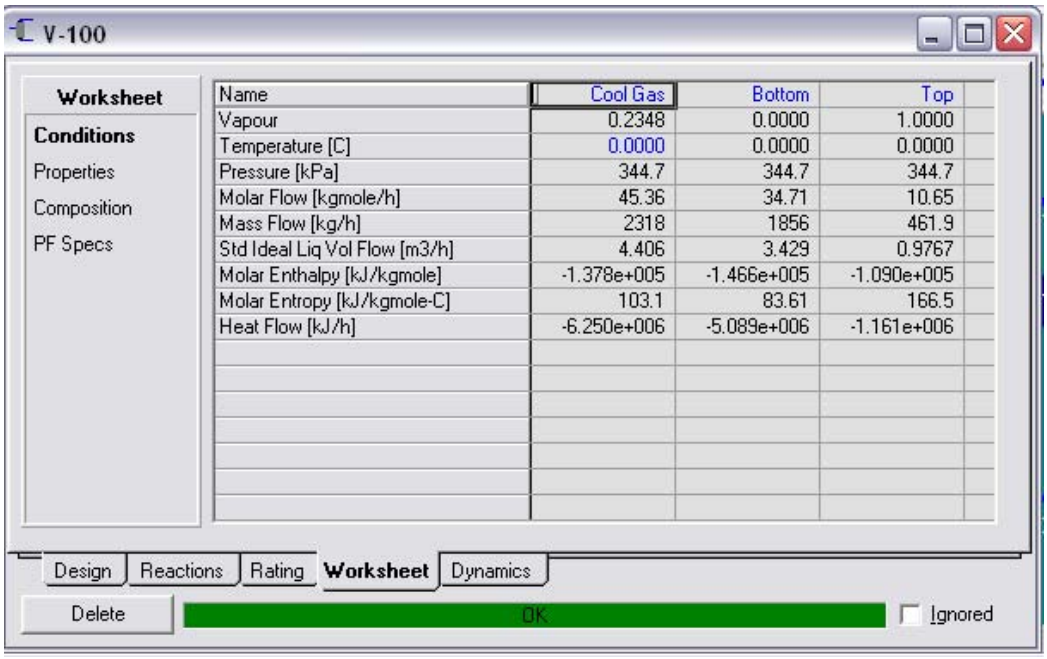


Figure 7-7

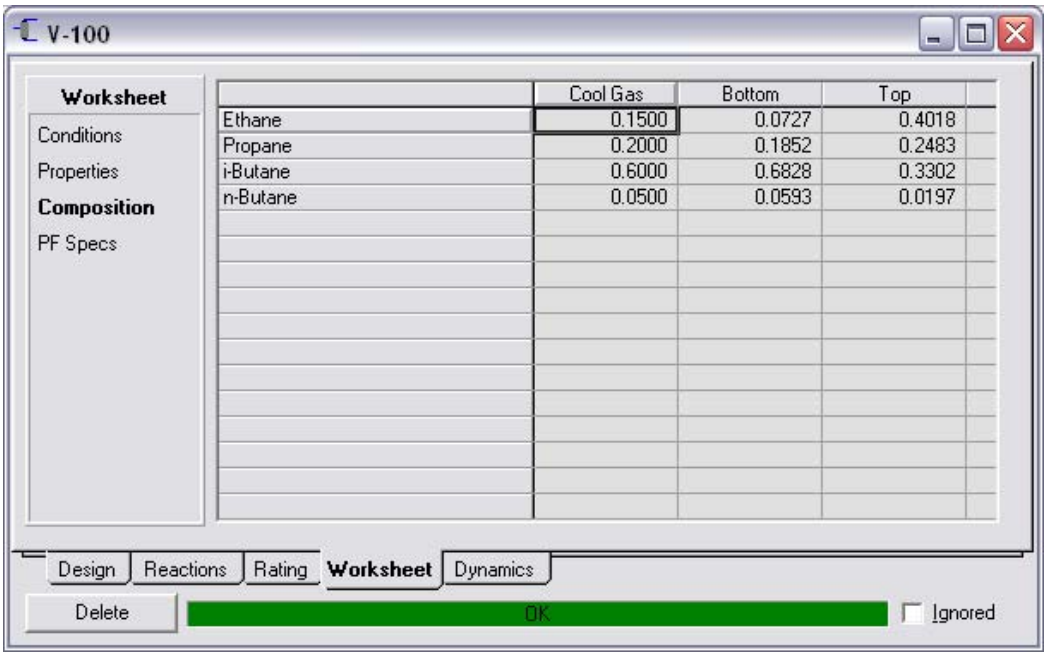


Figure 7-8

Stream:	Top	Bottom
Flowrate:	_____	_____
Composition:	Ethane: _____	_____
	Propane: _____	_____
	i-Butane: _____	_____
	n-Butane: _____	_____

7.7 Save Your Case

1. Go to the **File** menu.
2. Select **Save As**.
3. Give the HYSYS file the name **Flash** then press the OK button.

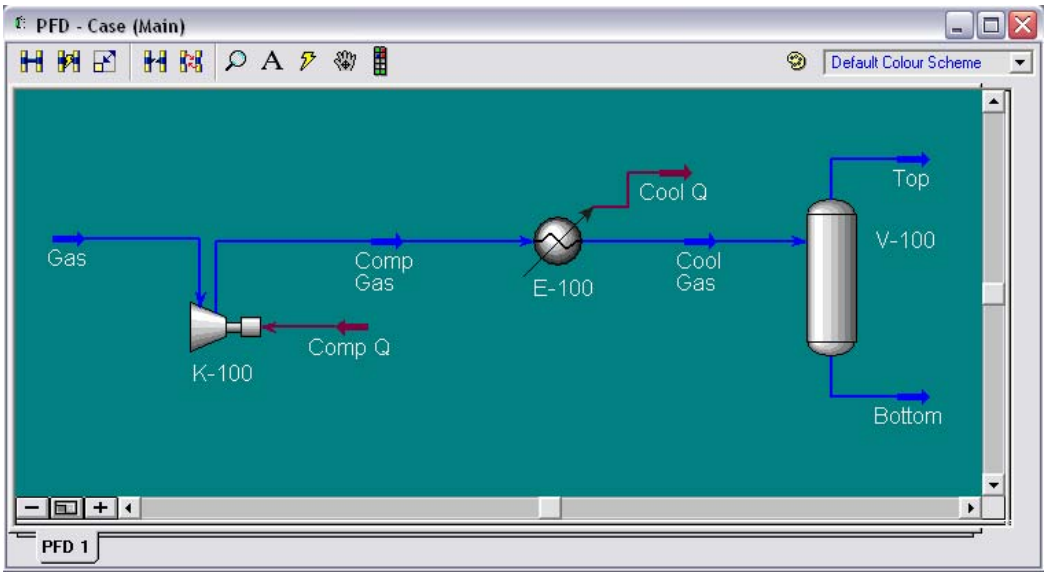


Figure 7-9

7.8 Review and Summary

In this chapter, the user was asked to find the flowrate of the liquid and vapor outlet streams of the flash separator. The vapor and liquid in the flash drum are allowed to reach equilibrium, before they are separated. HYSYS' separator was used to model the flash separation process.

7.9 Further Study

If the Cool Gas temperature is 10^{o}F, what are the new flowrates and compositions of these two streams?

Chapter 8
Conversion Reaction

Conversion Reaction

This chapter begins with a problem to develop a model that represents the partial oxidation reaction of methane to produce hydrogen. The partial oxidation method relies on the reaction of the methane with air in order to produce carbon oxides and hydrogen. The user will learn how to add the conversion reactions and reactions sets in HYSYS.

This reaction type does not require any thermodynamic knowledge. You must input the stoichiometry and the conversion of the basis reactant. The specified conversion cannot exceed 100%. The reaction will proceed until either the specified conversion has been reached or a limiting reagent has been exhausted.

Conversion reactions may not be grouped with any other form of reaction in a reaction set. However, they may be grouped with other conversion reactions and ranked to operate either sequentially or simultaneously. Lowest ranking occurs first (may start with either 0 or 1). Just as with single reactions, simultaneous reactions cannot total over 100% conversion of the same basis.

Conversion reactions cannot be used with Plug Flow Reactors or CSTRs. In general, they should only be used in Conversion Reactors.

Learning Outcomes: At the end of this chapter, the user will be able to:

- Simulate conversion reactor and reactions in HYSYS
- Add the reactions and reaction sets
- Attach reaction sets to the fluid package

Prerequisites: Before beginning this chapter, the users need to know how to:

- Navigate the PFD
- Add Streams in the PFD or the Workbook
- Add and connect Unit Operations

8.1 Problem Statement

The interest in production of hydrogen from hydrocarbons has grown significantly in the last decade. Efficient production of hydrogen is an enabling technology, directly related to the fuel cell energy conversion device. The conversion of fuels to hydrogen can be carried out by the partial oxidation. The partial oxidation method relies on the reaction of the fuel for example methane with air in order to produce carbon oxides and hydrogen.

$$CH_4 + \frac{1}{2}O_2 \rightarrow CO + 2H_2$$

$$CH_4 + O_2 \rightarrow CO_2 + 2H_2$$

Develop a model that represents partial oxidation of methane to produce hydrogen.

8.2 Defining the Simulation Basis

1. The first step in simulating a hydrogen production is choosing an appropriate fluid package. Enter the following values in the specified fluid package view:

On this page…	Select…
Property Package	Peng-Robinson
Components	CH_4, O_2, N_2, CO, CO_2, H_2

8.3 Adding the Reactions

Reactions in HYSYS are added in a manner very similar to the method used to add components to the simulation:

1. Click on the **Reactions** tab in the **Simulation Basis Manager** view. Note that all of the components are shown in the **Rxn Components** list.

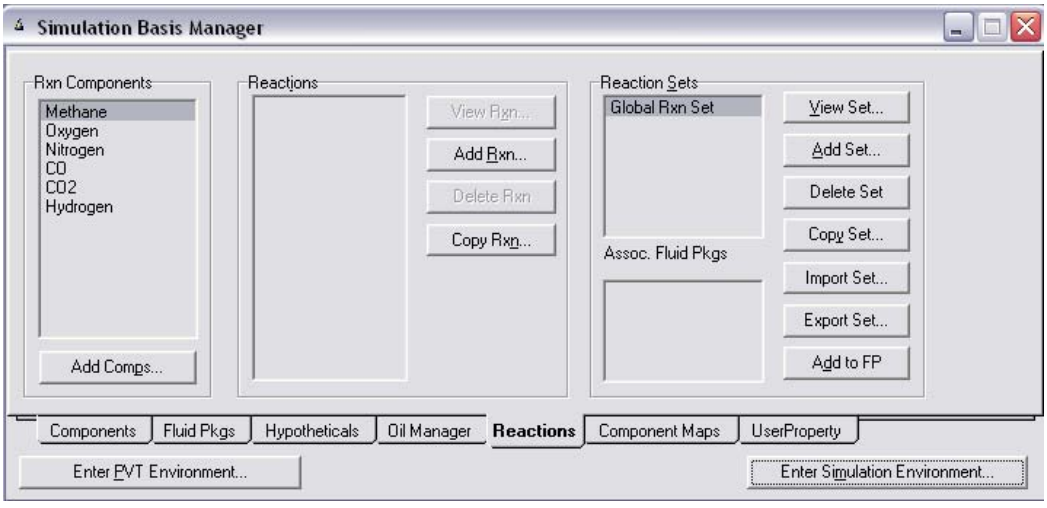


Figure 8-1

2. Click the **Add Rxn** button, and choose **Conversion** as the type from the displayed list. Enter the necessary information as shown:

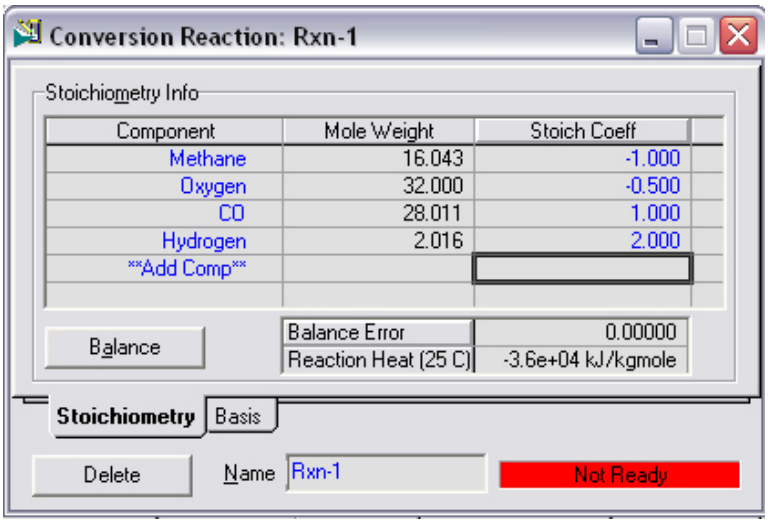


Figure 8-2

3. Move to the **Basis** tab and enter the information as shown:

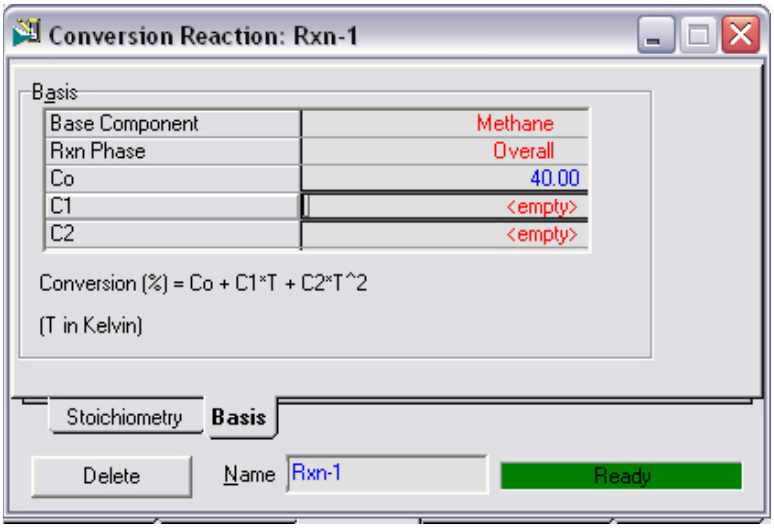


Figure 8-3

4. For the second reaction, enter the information as shown:

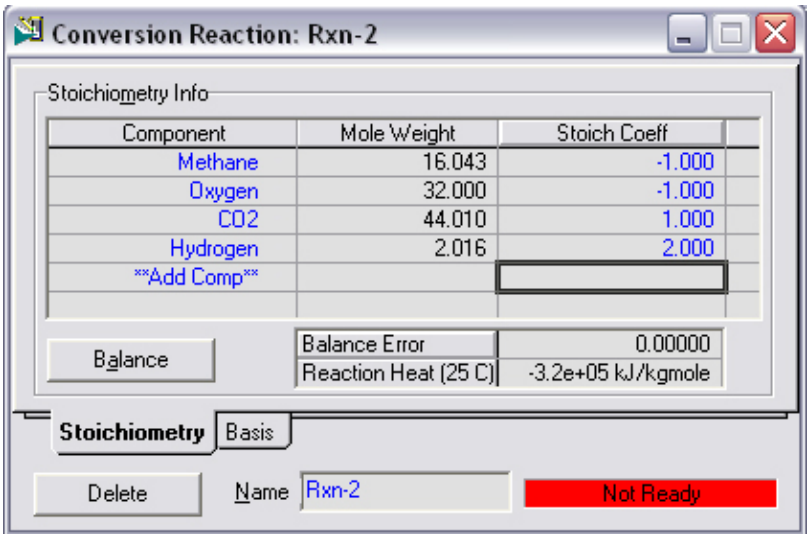


Figure 8-4

5. Move to the **Basis** tab and enter the information as shown:

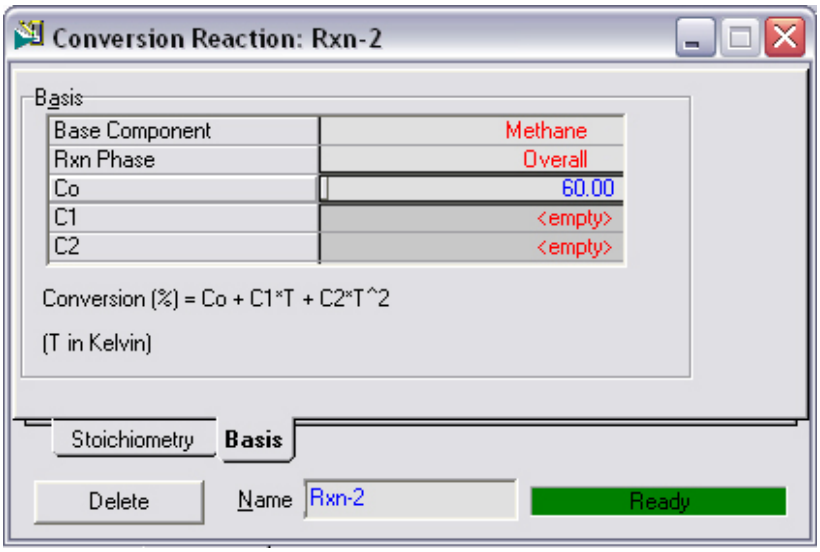


Figure 8-5

8.4 Adding the Reaction Sets

Once all two reactions are entered and defined, you can create a reaction set for the conversion reactor.

1. Still on the **Reactions** tab, click the **Add Set** button. Call the reaction set **Oxidation Rxn Set**, and add **Rxn-1** and **Rxn-2**. Reactions are added by highlighting the **<empty>** field in the **Active List** group, and selecting the desired reaction from the drop down list. The view should look like this after you are finished:

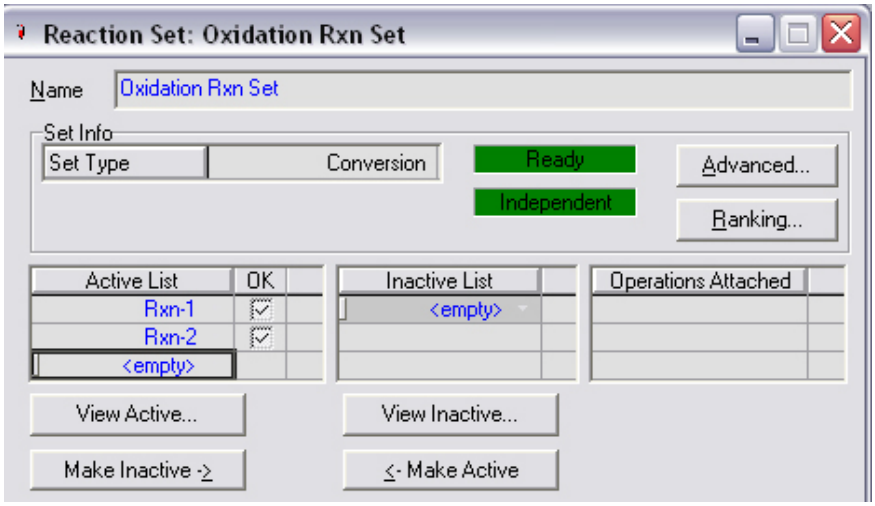


Figure 8-6

8.5 Making Sequential Reactions

Conversion reactions can be grouped with other conversion reactions and ranked to operate either sequentially or simultaneously. Lowest ranking occurs first (may start with either 0 or 1).

1. To make the reactions operate sequentially, in the **Oxidation Rxn Set**, click the **Ranking…** and enter the information as shown:

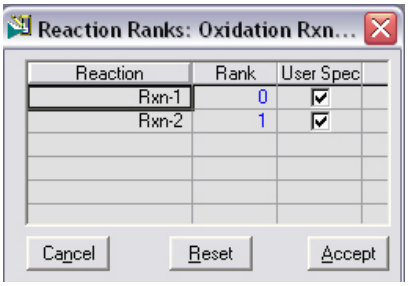


Figure 8-7

8.6 Attaching Reaction Set to the Fluid Package

After the reaction set has been created, it must be added to the current fluid package in order for HYSYS to use them.

1. Highlight the desired Reaction Set and press **Add to FP**.
2. Select the only available Fluid Package and press the **Add Set to Fluid Package** button.
3. If desired, you can save the Fluid Package with the attached reaction sets. This will allow you to reopen this FP in any number of HYSYS simulations.

Once the reaction set is added to the Fluid Package, you can enter the Simulation Environment and begin construction of the simulation.

8.7 Adding a Feed Stream

Add a new **Material** stream with the following values.

In this cell…	Enter…
Name	Methane
Temperature	25°C
Pressure	2 bar
Molar Flow	100 kgmole/h
Component Mole Fraction	
C_1	1.000

Add another new **Material** stream with the following values.

In this cell…	Enter…
Name	Air
Temperature	25°C
Pressure	2 bar
Molar Flow	260 kgmole/h
Component Mole Fraction	
N_2	0.790
O_2	0.210

8.8 Adding the Conversion Reactor

1. From the Object Palette, click **General Reactors.** Another palette appears with four reactor types: Gibbs, Equilibrium, Conversion and Yield. Select the **Conversion Reactor**, and enter it into the PFD.

Conversion Reactor icon

2. Name this reactor **Oxidation Reactor** and attach **Methane** and **Air** as feeds. Name the vapor outlet **Ox_Vap** and even though the liquid product from this reactor will be zero, we still must name the stream. Name the liquid product stream as **Ox_Liq**.

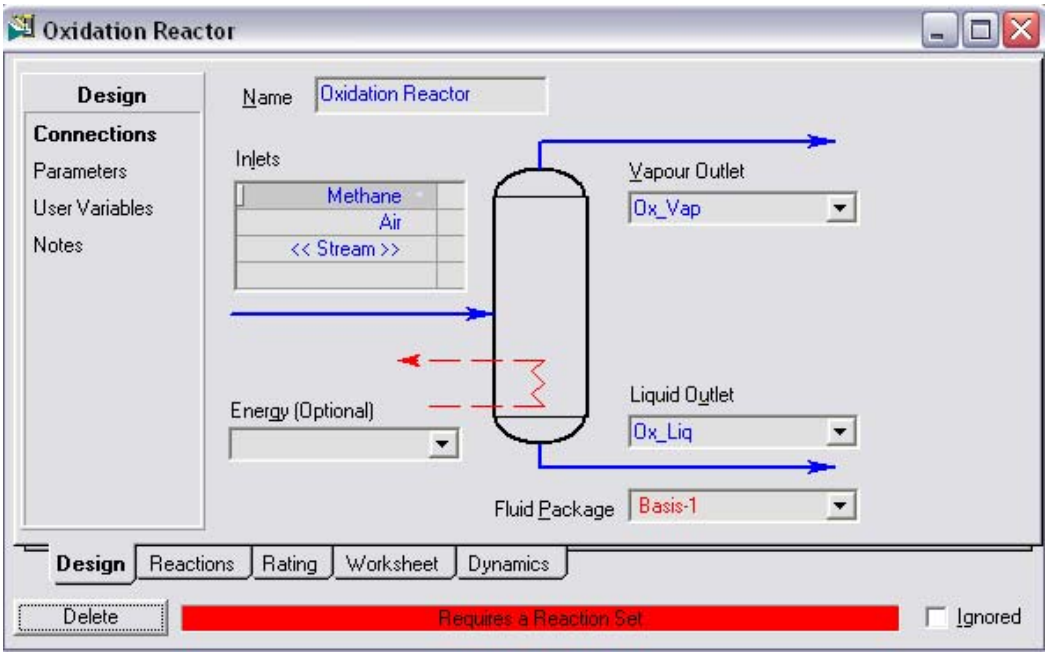


Figure 8-8

3. On the **Details** page of the **Reactions** tab, select **Oxidation Rxn Set** as the reaction set. This will automatically connect the proper reactions to this reactor.

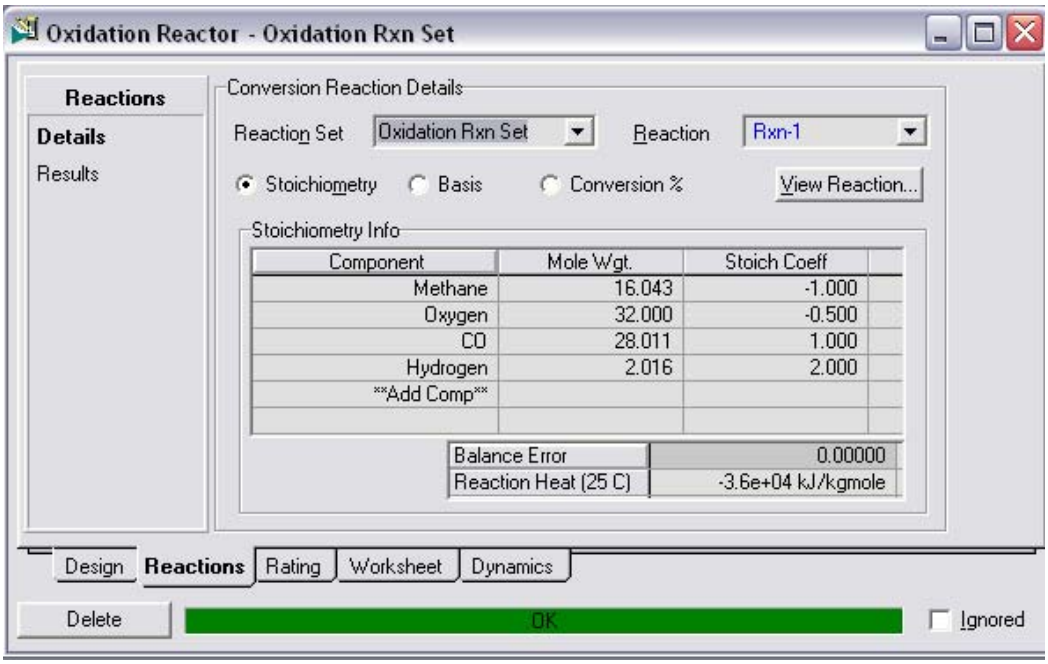


Figure 8-9

4. Go to the **Worksheet** tab. On the **Composition** page, analyze the composition in the **Ox_Vap** stream.

What is the molar flow of the following components?

Methane: _____ Nitrogen: _____

Oxygen: _____ CO: _____

CO2: _____ Hydrogen: _____

8.9 Save Your Case

1. Go to the **File** menu.
2. Select **Save As**.
3. Give the HYSYS file the name **Conversion** then press the OK button.

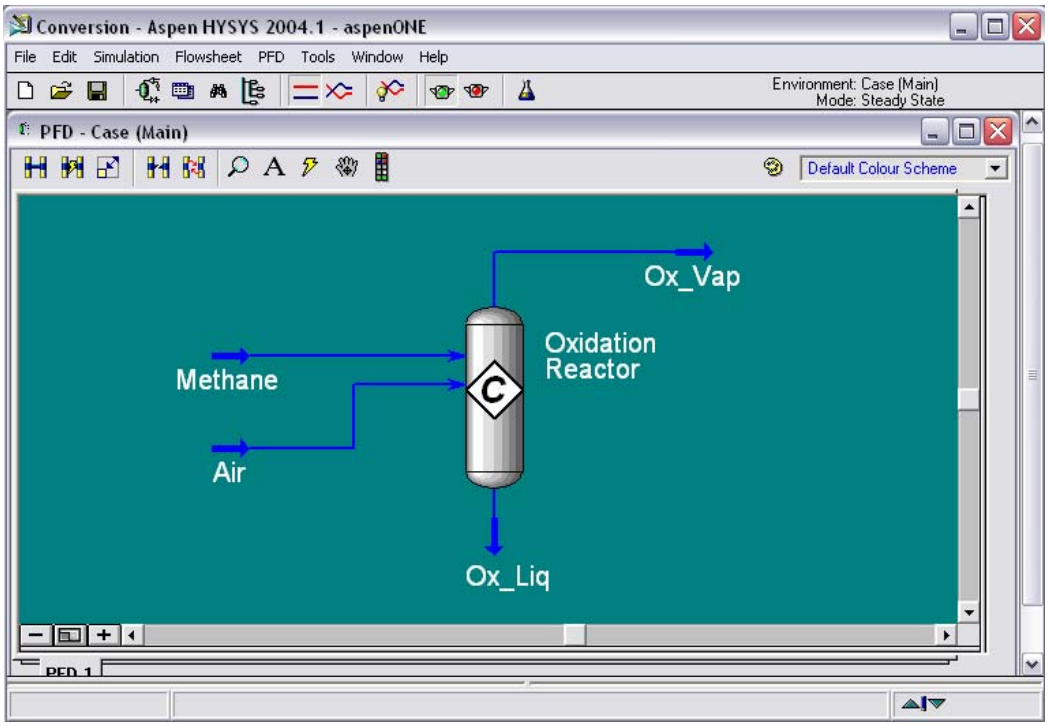


Figure 8-10

8.10 Review and Summary

In the first part of this chapter, we started with a problem to develop a model that represents the partial oxidation reaction of methane to produce hydrogen. The partial oxidation method relies on the reaction of the methane with air in order to produce carbon oxides and hydrogen. The user also learns how to add the conversion reactions and reactions sets in HYSYS.

Chapter 9
Equilibrium Reaction

Equilibrium Reaction

This chapter begins with a problem to develop a model that represents the water gas shift reaction. The role of the WGS reaction is to increase the H_2 yield and decrease the CO concentration to cell requirements to prevent the anode being poisoned and the cell efficiency abruptly drops. The user will learn how to add the equilibrium reactions and reactions sets in HYSYS.

The Equilibrium reactor is a vessel which models equilibrium reactions. The outlet streams of the reactor are in a state of chemical and physical equilibrium. The reaction set which you attach to the Equilibrium reactor can contain an unlimited number of equilibrium reactions, which are simultaneously or sequentially solved. Neither the components nor the mixing process need be ideal, since HYSYS can compute the chemical activity of each component in the mixture based on mixture and pure component fugacities.

You can also examine the actual conversion, the base component, the equilibrium constant, and the reaction extent for each reaction in the selected reaction set. The conversion, the equilibrium constant and the extent are all calculated based on the equilibrium reaction information which you provided when the reaction set was created.

Learning Outcomes: At the end of this chapter, the user will be able to:

- Simulate equilibrium reactor and reactions in HYSYS
- Re-add the reactions and reaction sets
- Attach reaction sets to the fluid package
- Print Stream and Workbook Datasheets

Prerequisites: Before beginning this chapter, the users need to know how to:

- Navigate the PFD
- Add Streams in the PFD or the Workbook
- Add and connect Unit Operations

9.1 Problem Statement

The new application of hydrogen as a raw material for fuel cells for mobile power sources (PEM fuel cells) requires that the anode inlet gas have a CO concentration lower than 10-20 ppm. Otherwise, the anode is poisoned and the cell efficiency abruptly drops.

Hence, if the hydrogen is produced from hydrocarbon or alcohol reforming, purification is required in order to reduce the CO levels to cell requirements. The most technologically feasible purification train consists of a water gas shift reaction (WGS). The reaction

$$CO + H_2O \leftrightarrow CO_2 + H_2$$

has been employed for 40 years in the industrial process for H_2 production from liquid and gaseous hydrocarbons. The role of the WGS reaction is to increase the H_2 yield and decrease the CO concentration, which is a poison for some catalysts used.

Develop a model that represents the water gas shift reaction.

9.2 Defining the Simulation Basis

1. For this chapter, you will be using the saved case from the previous chapter (Chapter 8: Conversion Reaction) with one additional component, **H_2O**.
2. Open the previous simulation case: **Conversion**.

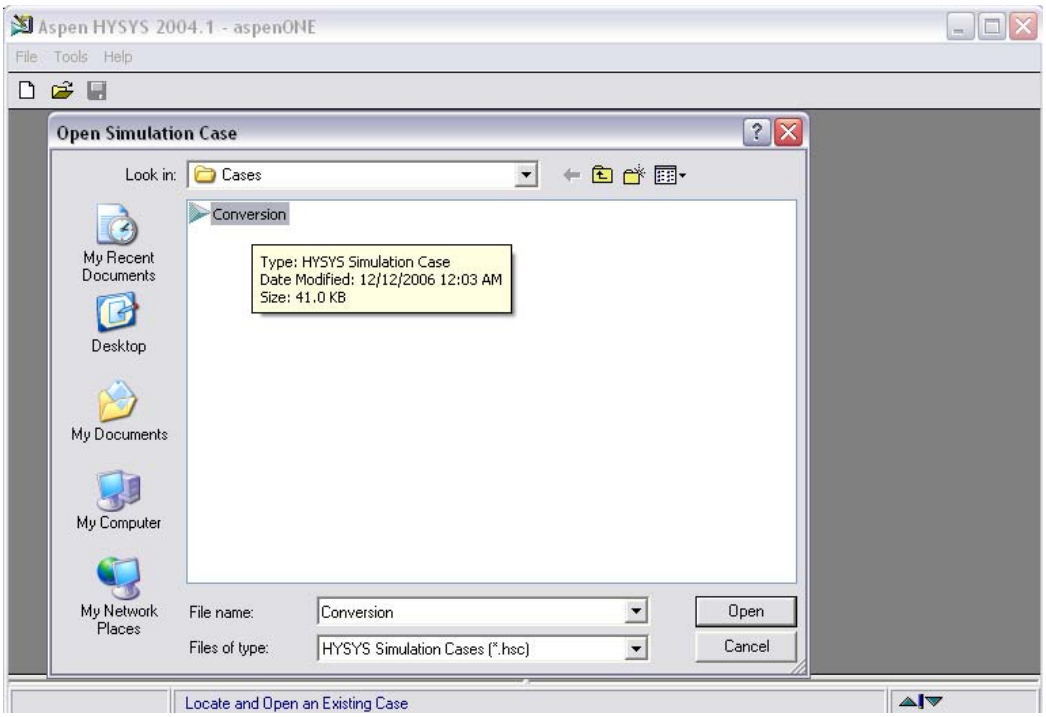


Figure 9-1

3. Click the **Enter Basis Environment** button to view the **Simulation Basis Manager**.
4. In the **Components** tab, **View** the **Component List-1** to add new component.
5. Add H_2O to the list as shown the following figure.

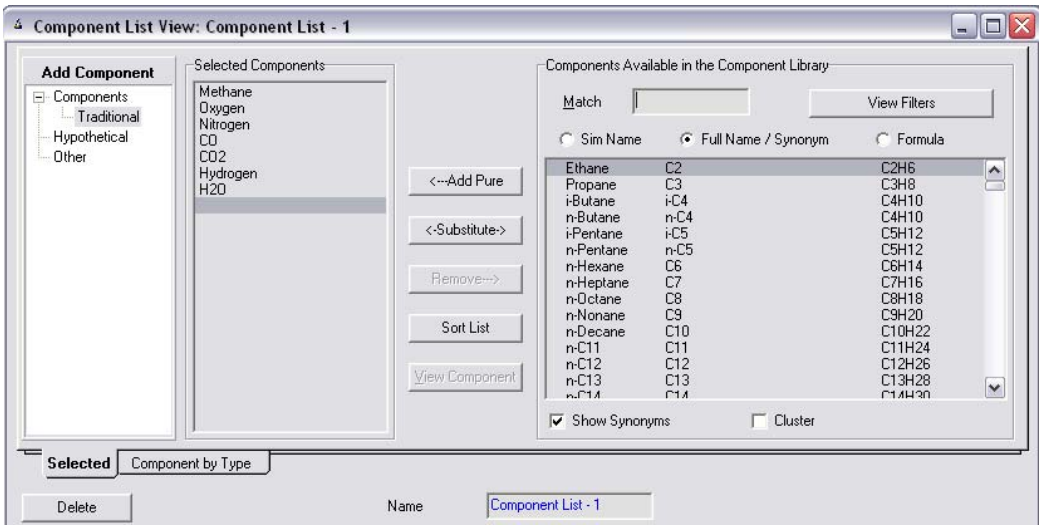


Figure 9-2

9.3 Adding the Reactions

Reactions in HYSYS are added in a manner very similar to the method used to add components to the simulation:

1. Click on the **Reactions** tab in the **Simulation Basis Manager** view. Note that all of the components are shown in the **Rxn Components** list.

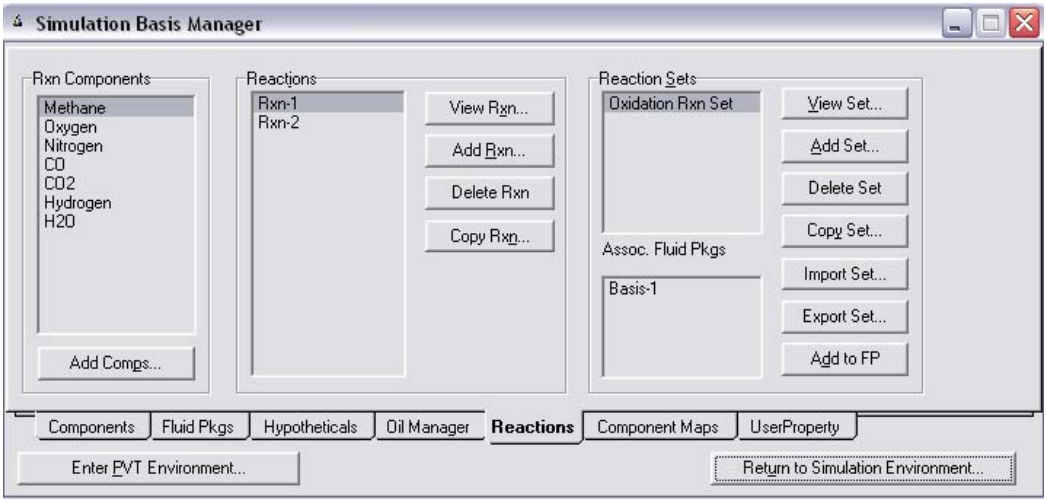


Figure 9-3

2. Click the **Add Rxn** button, and choose **Equilibrium** as the type from the displayed list. Enter the necessary information as shown:

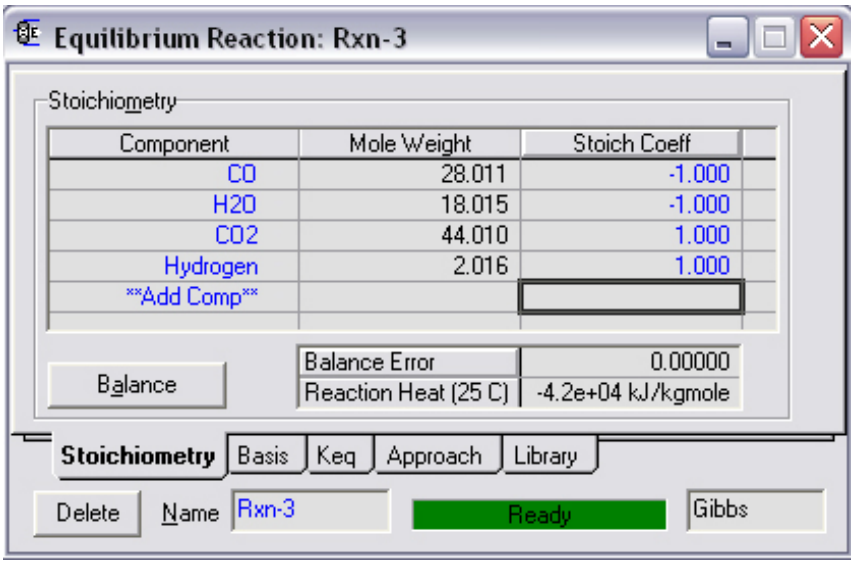


Figure 9-4

9.4 Adding the Reaction Sets

Once the reaction is entered and defined, you can create a reaction set for the equilibrium reactor.

1. Still on the **Reactions** tab, click the **Add Set** button. Call the reaction set **WGS Rxn Set**, and add **Rxn-3**. Reactions are added by highlighting the **<empty>** field in the **Active List** group, and selecting the desired reaction from the drop down list. The view should look like this after you are finished:

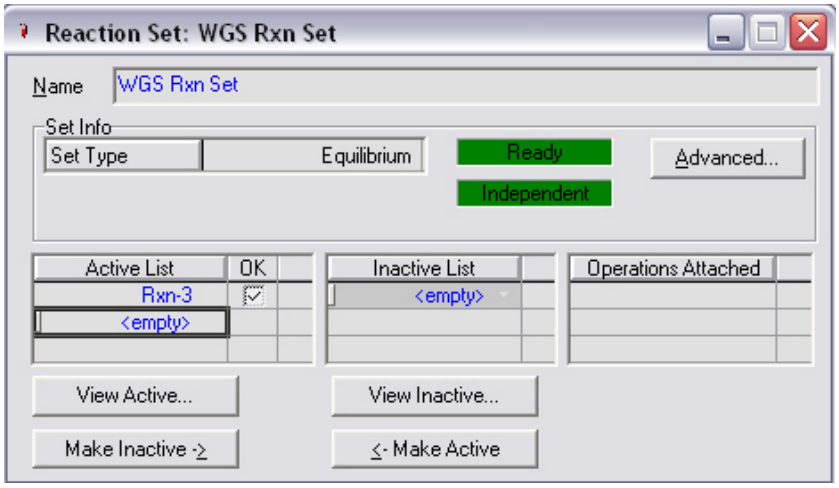


Figure 9-5

9.5 Attaching Reaction Set to the Fluid Package

After the reaction set has been created, it must be added to the current fluid package in order for HYSYS to use them.

1. Highlight the desired Reaction Set and press **Add to FP**.
2. Select the only available Fluid Package and press the **Add Set to Fluid Package** button.

Once the reaction set is added to the Fluid Package, Click **Return to the Simulation Environment** and begin construction of the simulation. Make sure the **Solver** is active.

9.6 Adding a Feed Stream

Add a new **Material** stream with the following values.

In this cell…	Enter…
Name	Steam
Temperature	100°C
Pressure	2 bar
Molar Flow	100 kgmole/h
Component Mole Fraction	
H_2O	1.000

9.7 Adding the Equilibrium Reactor

1. From the Object Palette, click **General Reactors.** Another palette appears with four reactor types: Gibbs, Equilibrium, Conversion and Yield. Select the **Equilibrium Reactor**, and enter it into the PFD.
2. Name this reactor **WGS Reactor** and attach **Ox_Vap** and **Steam** as feeds. Name the vapor outlet **WGS_Vap** and even though the liquid product from this reactor will be zero, we still must name the stream. Name the liquid product stream as **WGS_Liq**.

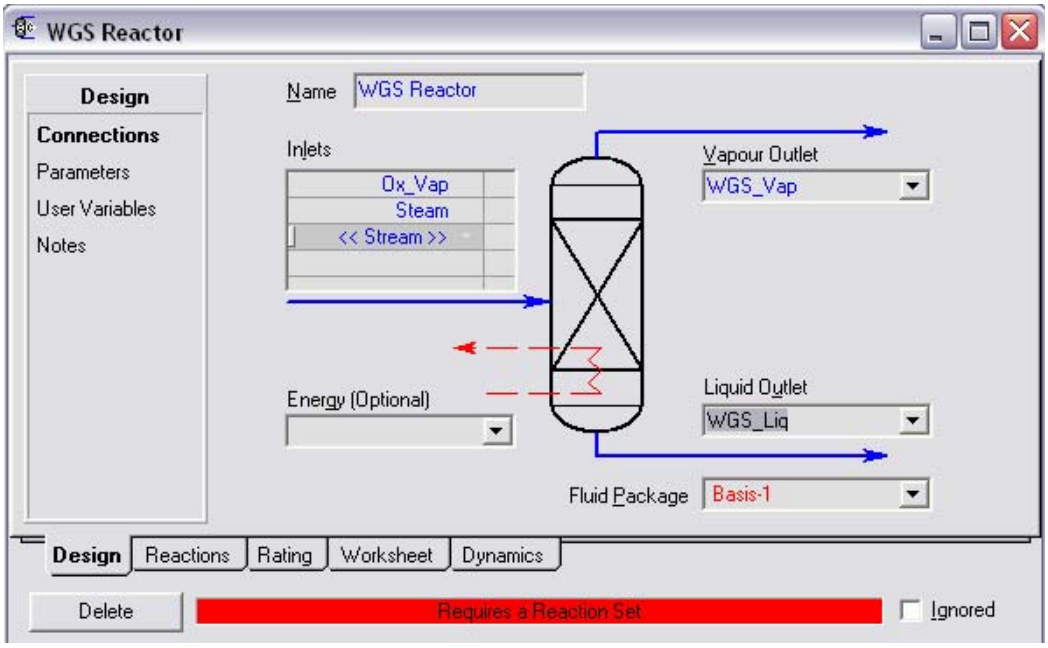


Figure 9-6

3. On the **Details** page of the **Reactions** tab, select **WGS Rxn Set** as the reaction set. This will automatically connect the proper reactions to this reactor.

Figure 9-7

4. Go to the **Worksheet** tab. On the **Composition** page, analyze the composition in the **WGS_Vap** stream.

What is the molar flow of the following components?

Methane: _____ Nitrogen: _____

Oxygen: _____ CO: _____

CO2: _____ Hydrogen: _____

Calculate the percentages of the following (compare results from Chapter 8):

CO reduced: _____

Hydrogen increased: _____

9.8 Printing Stream and Workbook Datasheets

In Aspen HYSYS you have the ability to print Datasheets for streams, operations, and workbooks.

1. Open the Workbook. Go to **Tools** > **Workbook** (or **Ctrl+W**). Workbook will be shown as in Figure 9.8.
2. Insert the mole fraction of all components to the Workbook. Go to **Workbook** > **Setup**.

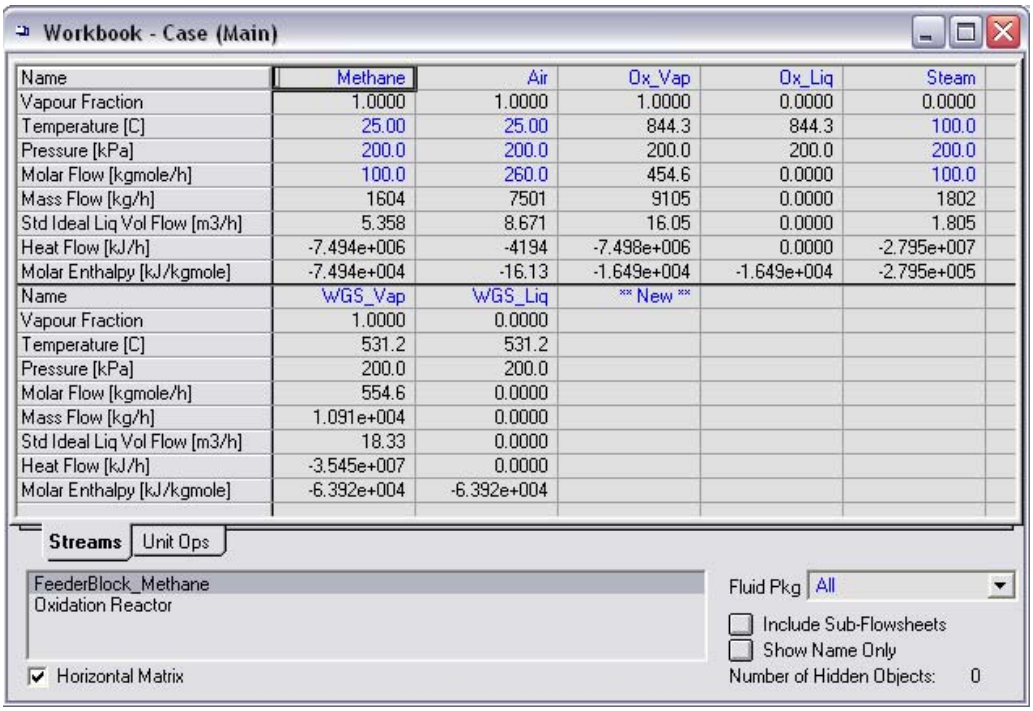


Figure 9-8

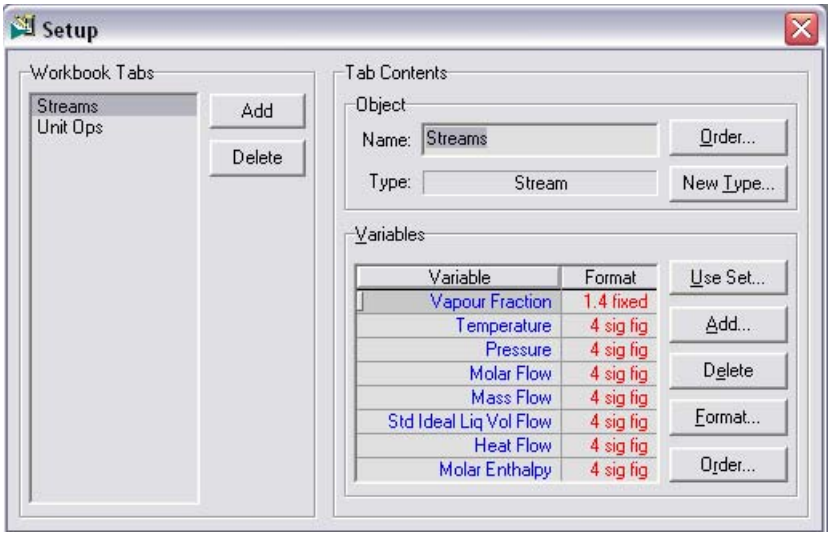


Figure 9-9

3. In the **Variables** page, click **Add…**, and Figure 9-10 will be shown.
4. In the **Variable** page, select **Master Comp Molar Flow** and in the **Variable Specifics**, select **Methane**. Click **OK**.

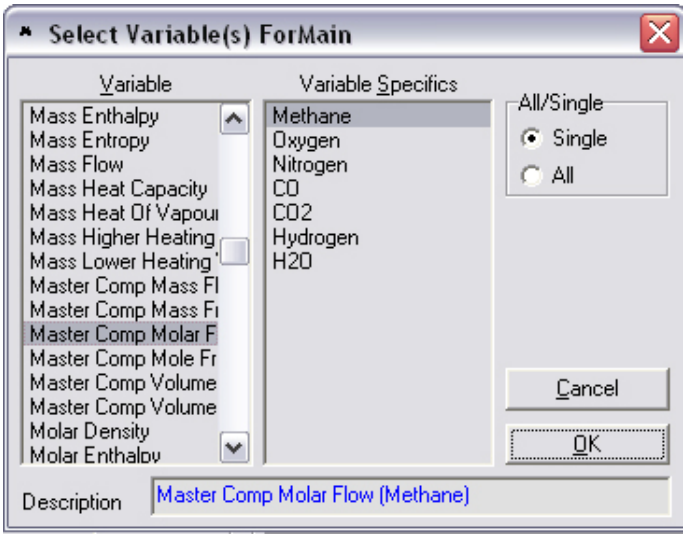


Figure 9-10

5. Repeat step 4 to insert all components. Once finished, preview the Workbook as shown in Figure 9-11.

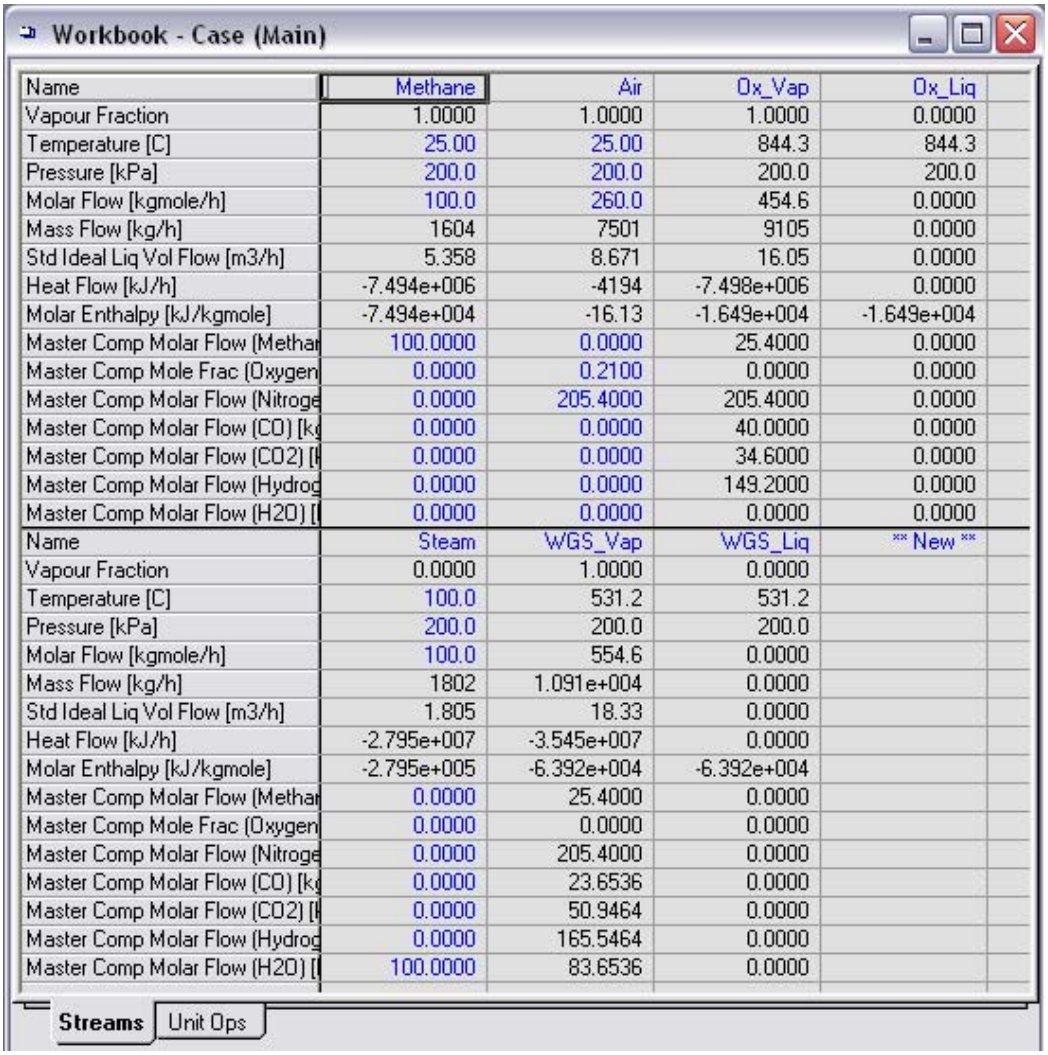


Figure 9-11

6. Right-click (object inspect) the Workbook title bar. The **Print Datasheet** pop-up menu displays.

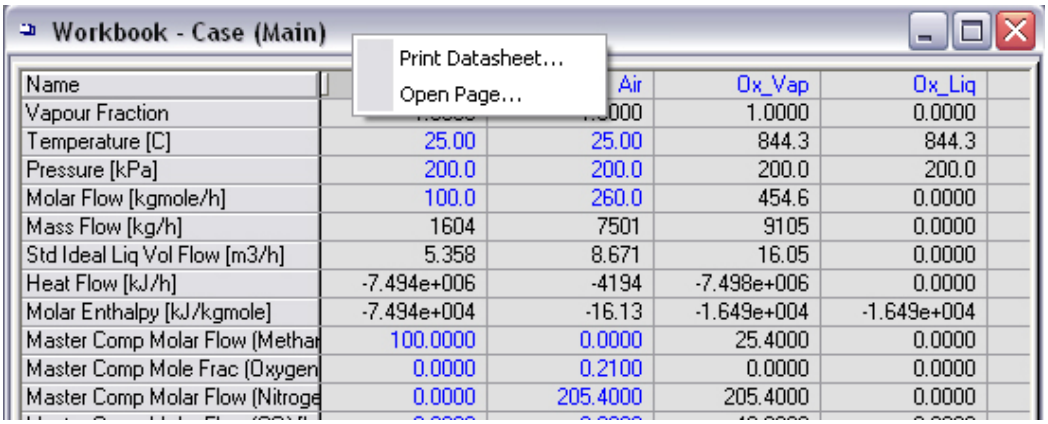


Figure 9-12

7. Select **Print Datasheet**. The **Select Datablock** view displays.

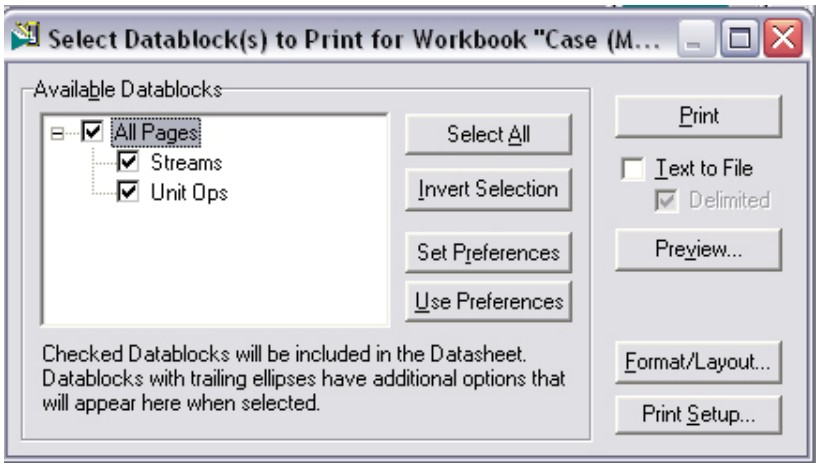


Figure 9-13

8. From the list, you can choose to print or preview any of the available datasheets.

9.9 Save Your Case

1. Go to the **File** menu.
2. Select **Save As**.
3. Give the HYSYS file the name **Equilibrium** then press the OK button.

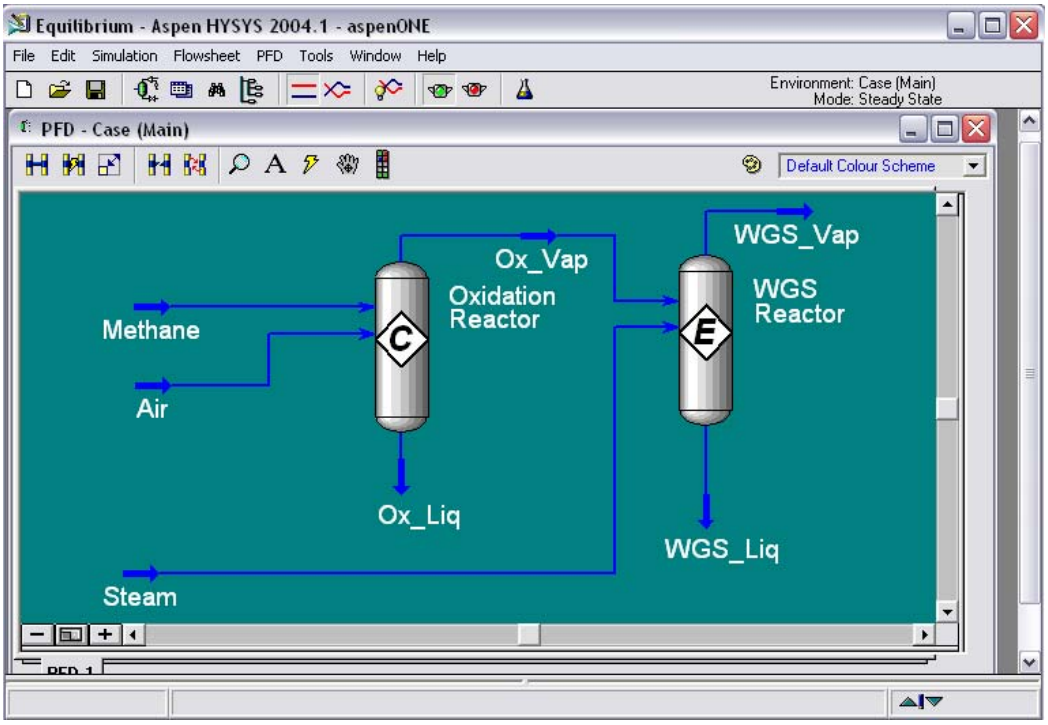


Figure 9-14

9.10 Review and Summary

In the first part of this chapter, we started with a problem to develop a model that represents the water gas shift reaction. The role of the WGS reaction is to increase the H_2 yield and decrease the CO concentration to cell requirements to prevent the anode being poisoned and the cell efficiency abruptly drops. The user also learns how to add the equilibrium reactions and reactions sets in HYSYS.

Chapter 10
CSTR

CSTR

In this chapter, a flowsheet for the production of propylene glycol is presented. Propylene oxide is combined with water to produce propylene glycol in a continuously-stirred-tank reactor (CSTR).

The propylene oxide and water feed streams are combined in a mixer. The combined stream is fed to a reactor, operating at atmospheric pressure, in which propylene glycol is produced.

Learning Outcomes: At the end of this chapter, the user will be able to:

- Simulate continuously-stirred-tank reactor and reactions in HYSYS
- Set new Session Preferences

Prerequisites: Before beginning this chapter, the users need to know how to:

- Navigate the PFD
- Add Streams in the PFD or the Workbook
- Add and connect Unit Operations

10.1 Setting New Session Preferences

Start HYSYS and create a new case. Your first task is to set your Session Preferences.

1. From the **Tools** menu, select **Preferences**. The **Session Preferences** property view appears.

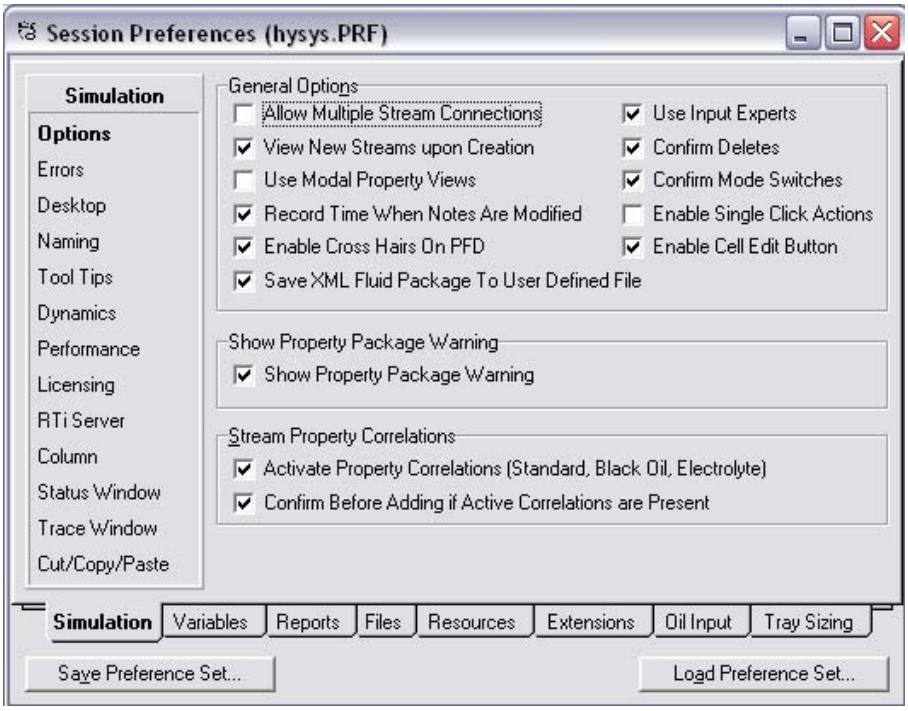


Figure 10-1

2. The **Simulation** tab, **Options** page should be visible. Ensure that the **Use Modal Property Views** checkbox is unchecked.
3. Click the **Variables** tab, then select the **Units** page.

10.2 Creating a New Unit Set

The first task you perform when building the simulation case is choosing a unit set. HYSYS does not allow you to change any of the three default unit sets listed, however, you can create a new unit set by cloning an existing one. For this chapter, you will create a new unit set based on the HYSYS Field set, then customize it.

1. In the **Available Units Set** list, select **Field**.
   The default unit for **Liq. Vol. Flow** is **barrel/day**; next you will change the **Liq. Vol. Flow** units to **USGPM**.

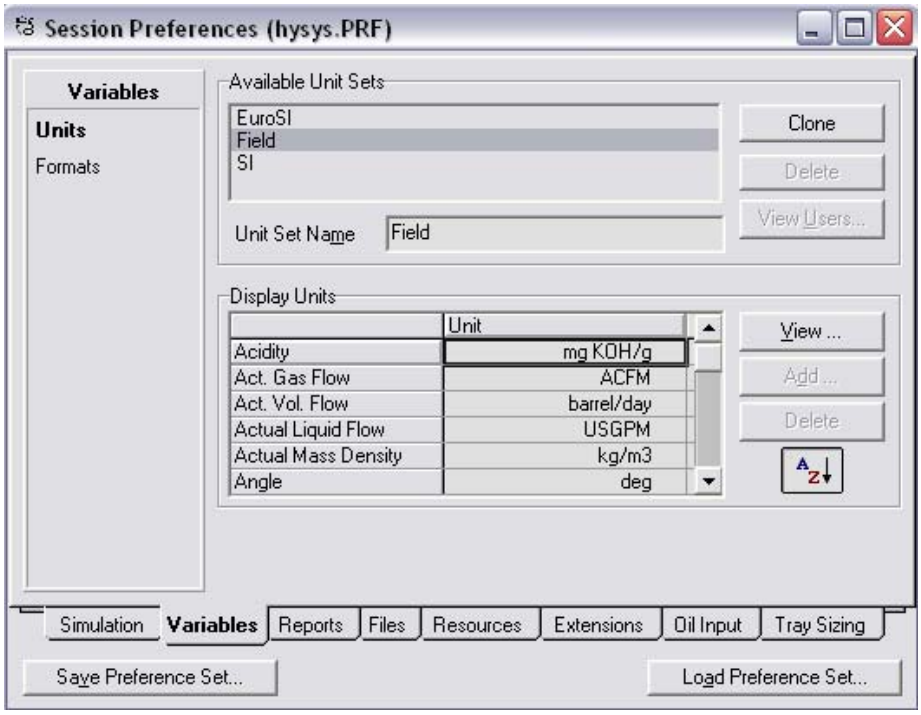


Figure 10-2

The default Preference file is named **HYSYS.prf**. When you modify any of the preferences, you can save the changes in a new Preference file by clicking the **Save Preference Set** button. HYSYS prompts you to provide a name for the new Preference file, which you can later recall into any simulation case by clicking the **Load Preference Set** button

2. Click the **Clone** button. A new set named **NewUser** appears in the **Available Unit Sets** list.
3. In the **Unit Set Name** filed, change the name to **Field-USGPM**. You can now change the units for any variable associated with this new unit set.
4. Find the **Liq. Vol. Flow** cell. Click in the **barrel/day** cell beside it.
5. To open the list of available units, click the down arrow, or press the **F2** key then the Down arrow key.
6. From the list, select **USGPM**.

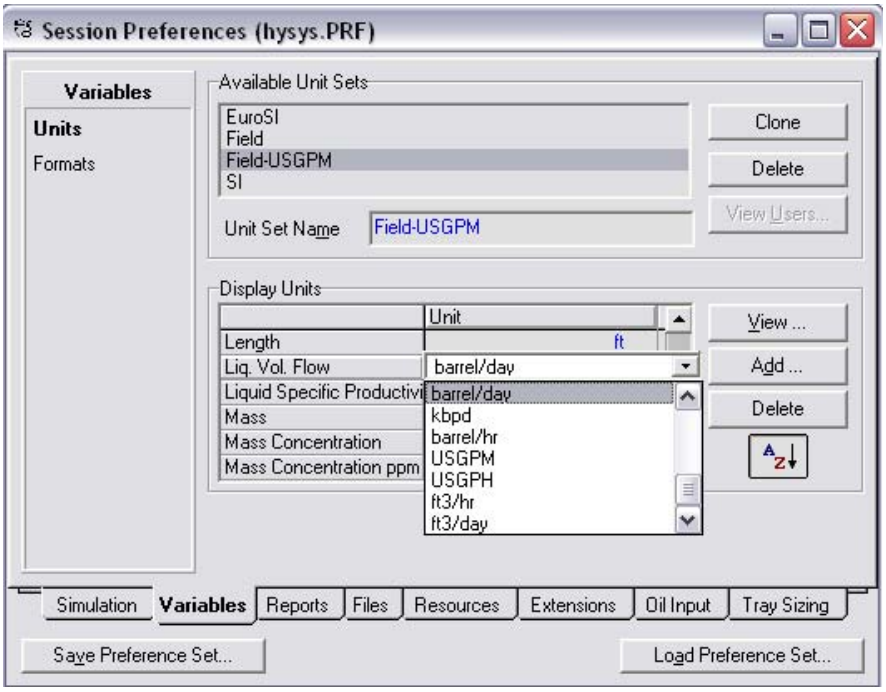


Figure 10-3

7. The new unit set is now defined. Close the Session Preferences property view.

10.3 Defining the Simulation

1. Enter the following values in the specified fluid package view:

On this page…	Select…
Property Package	UNIQUAC
Components	Propylene Oxide, Propylene Glycol, H_2O

10.4 Providing Binary Coefficients

The next task in defining the Fluid Package is providing the binary interaction parameters.

1. Click the **Binary Coeffs** tab of the Fluid Package property view.

Figure 10-4

In the Activity Model Interaction Parameters group, the Aij interaction table appears by default. HYSYS automatically inserts the coefficients for any component pairs for which library data is available. You can change any of the values provided by HYSYS if you have data of you own.

In this case, the only unknown coefficients in the table are for the 12C3Oxide/12-C3diol pair. You can enter these values if you have available data, however, here, you will use one of HYSYS's built-in estimation methods instead.

2. Next, you will use the **UNIFAC VLE** estimation method to estimate the unknown pair.
3. Click the **Unknowns Only** button. HYSYS provides values for the unknown pair. The final Activity Model Interaction Parameters table for the Aij coefficients appears below.

Figure 10-5

4. To view the Bij coefficient table, select the Bij radio button. For this case, all the **Bij** coefficients will be left at the default value of zero.

10.5 Defining the Reaction

1. Return to the Simulation Basis Manager
2. Click the **Reactions** tab. This tab allows you to define all the reactions for the flowsheet.
   The reaction between water and propylene oxide to produce propylene glycol is as follows:

$$H_2O + C_3H_6O \rightarrow C_3H_8O_2$$

   These steps will be followed in defining our reaction:

   i. Create and define a Kinetic Reaction.
   ii. Create a Reaction Set containing the reaction.
   iii. Activate the Reaction Set to make it available for use in the flowsheet.

10.6 Creating the Reaction

1. In the Reactions group, click the **Add Rxn** button. The reactions property view appears.
2. In the list, select the Kinetic reaction type, then click the Add Reaction button. The Kinetic Reaction property view appears, opened to the Stoichiometry tab. Enter the necessary information as shown:

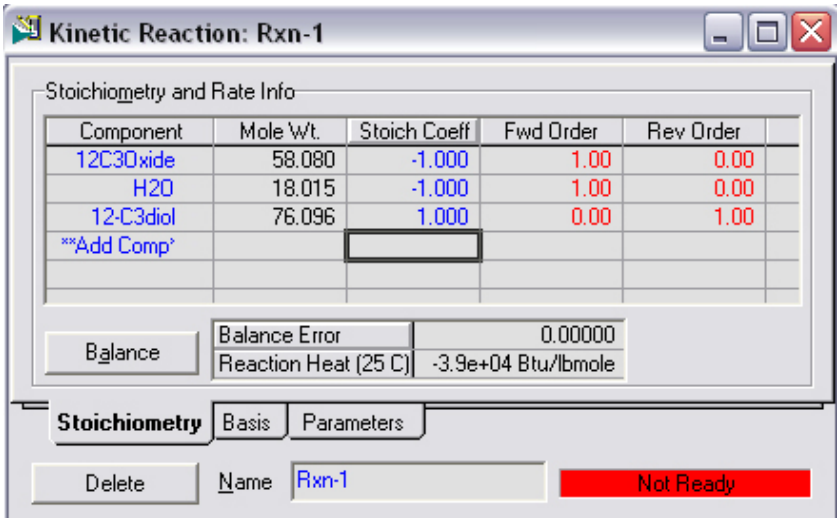


Figure 10-6

   HYSYS provides default values for the **Forward Order** and **Reverse Order** based on the reaction stoichiometry. The kinetic data for this case is based on an excess of water, so the kinetics are first order in **Propylene Oxide** only.
3. In the **Fwd Order** cell for **H2O**, change the value to **0** to reflect the excess of water. The stoichiometry tab is now completely defined and appears as shown below.

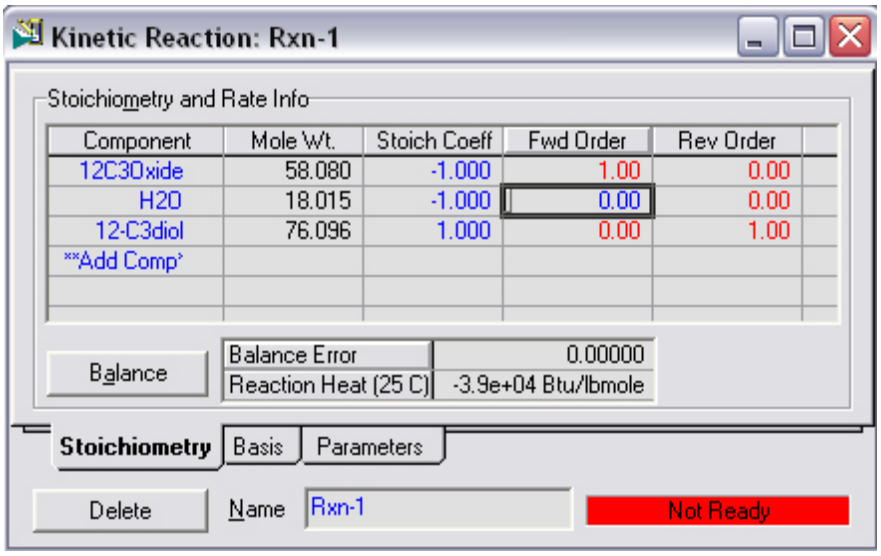


Figure 10-7

The next task is to define the reaction basis.

4. In the Kinetic Reaction property view, click the **Basis** tab.
5. In the **Basis** cell, accept the default value of **Molar Concn**.
6. Click in the **Base Component** cell. By default, HYSYS has chosen the first component listed on the **Stoichiometry** tab, in this case **Propylene oxide**, as the base component.
7. In the **Rxn Phase** cell, select **CombinedLiquid** from the drop-down list. The completed **Basis** tab appears below.

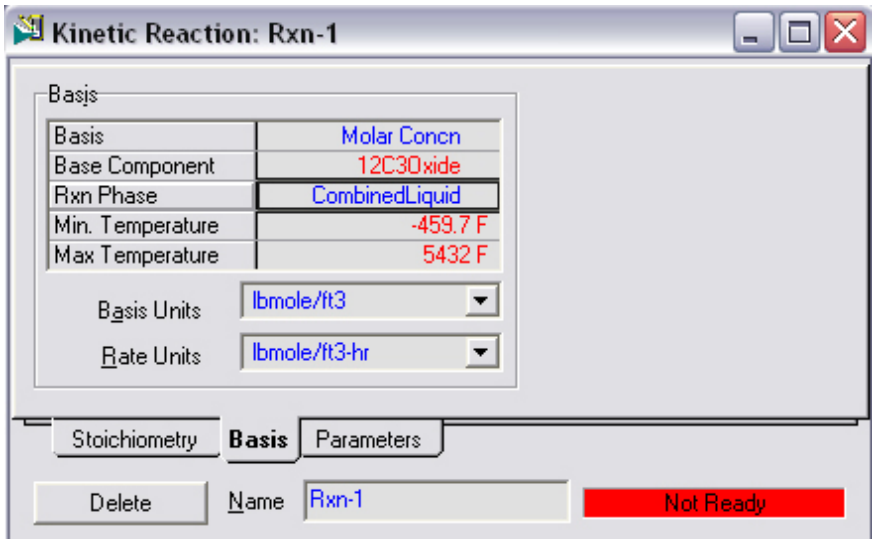


Figure 10-8

8. Click the **Parameters** tab. On this tab you provide the **Arrhenius** parameters for the kinetic reaction. In this case, there is no **Reverse Reaction** occurring, so you only need to supply the **Forward Reaction** parameters.
9. In the Forward Reaction **A** cell, enter **1.7e13**.
10. In the Forward Reaction **E** cell (activation energy), enter **3.24e4** (btu/lbmole). The status indicator at the bottom of the **Kinetic Reaction** property view changes from

Not Ready to **Ready**, indicating that the reaction is completely defined. The final **Parameters** tab appears below.

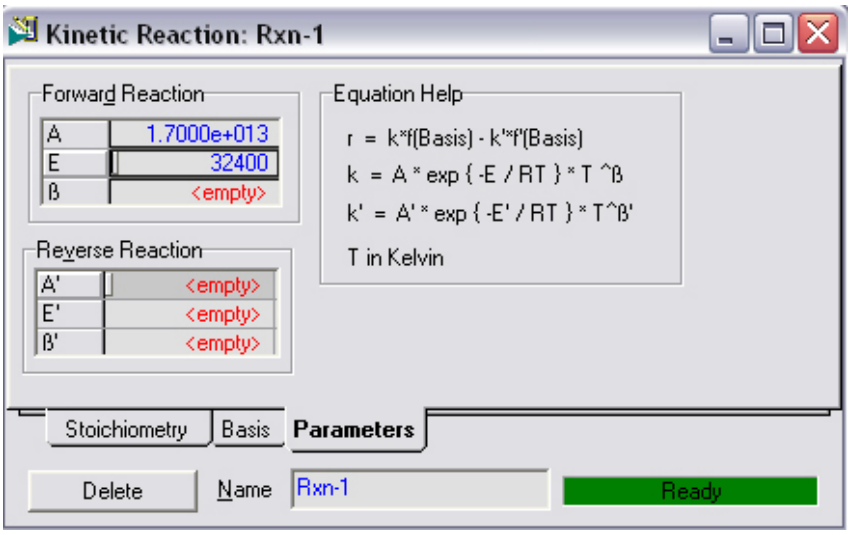


Figure 10-9

11. The next task is to create a reaction set that will contain the new reaction. In the Reaction Sets list, HYSYS provides the Global Rxn Set which contains all of the reactions you have defined. In this case, since there is only one reactor, the default Global Rxn Set could be attached to it. Add Rxn-1 to Global Rxn Set.
12. The final task is to make the set available to the Fluid Package, which also makes it available in the flowsheet. Add the Reaction Set to the Fluid Package. Once the reaction set is added to the Fluid Package, Click **Enter the Simulation Environment** and begin construction of the simulation.

10.7 Adding a Feed Stream

Add a new **Material** stream with the following values.

In this cell…	Enter…
Name	Prop Oxide
Temperature	75°F
Pressure	1.1 atm
Molar Flow	150 lbmole/h
Component Mole Fraction	
12C3Oxide	1.000

Add another new **Material** stream with the following values.

In this cell…	Enter…
Name	Water Feed
Temperature	75°F
Pressure	16.17 psia
Mass Flow	11,000 lb/h
Component Mole Fraction	
H2O	1.000

10.8 Installing Unit Operations

Now that the feed streams are known, your next task is to install the necessary unit operations for producing the glycol.

Installing the Mixer

The first operation is a **Mixer**, used to combine the two feed streams. Enter the necessary information as shown:

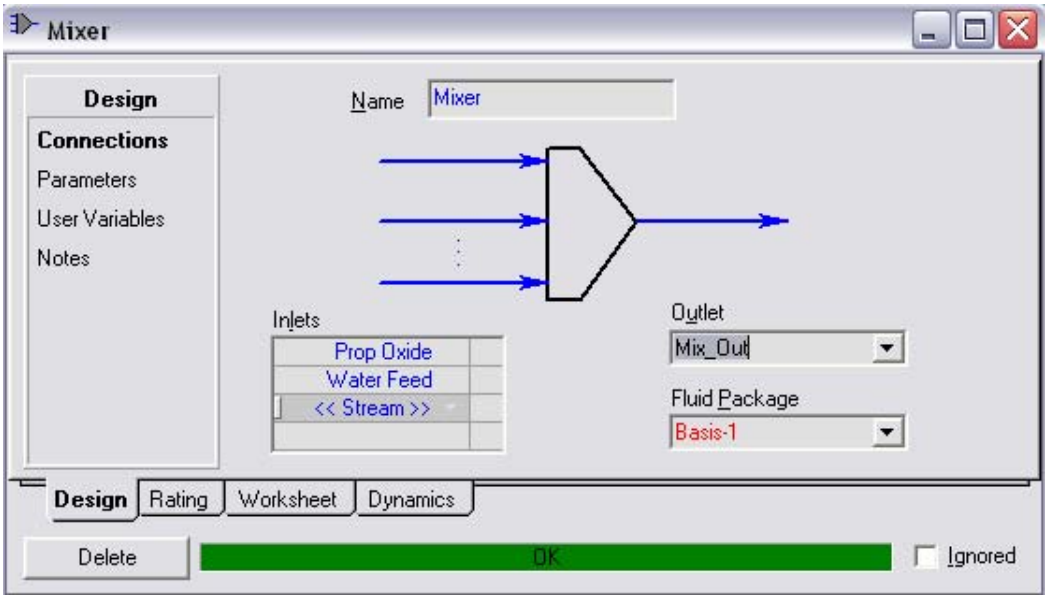


Figure 10-10

Installing the Reactor

1. From the Object Palette, click **CSTR**, and enter it into the PFD.
2. Name this reactor **CSTR** and attach **Mix_Out** as feed. Name the vapor outlet **CSTR Vent** and the liquid product stream as **CSTR Product**.

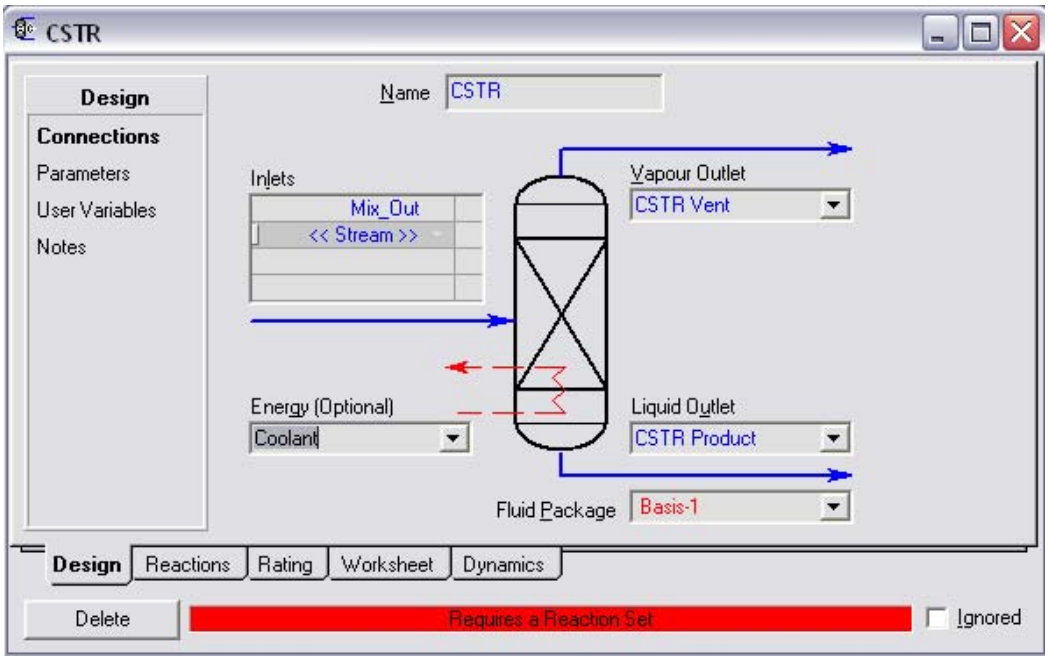


Figure 10-11

3. On the **Details** page of the **Reactions** tab, select **Global Rxn Set** as the reaction set. This will automatically connect the proper reactions to this reactor.

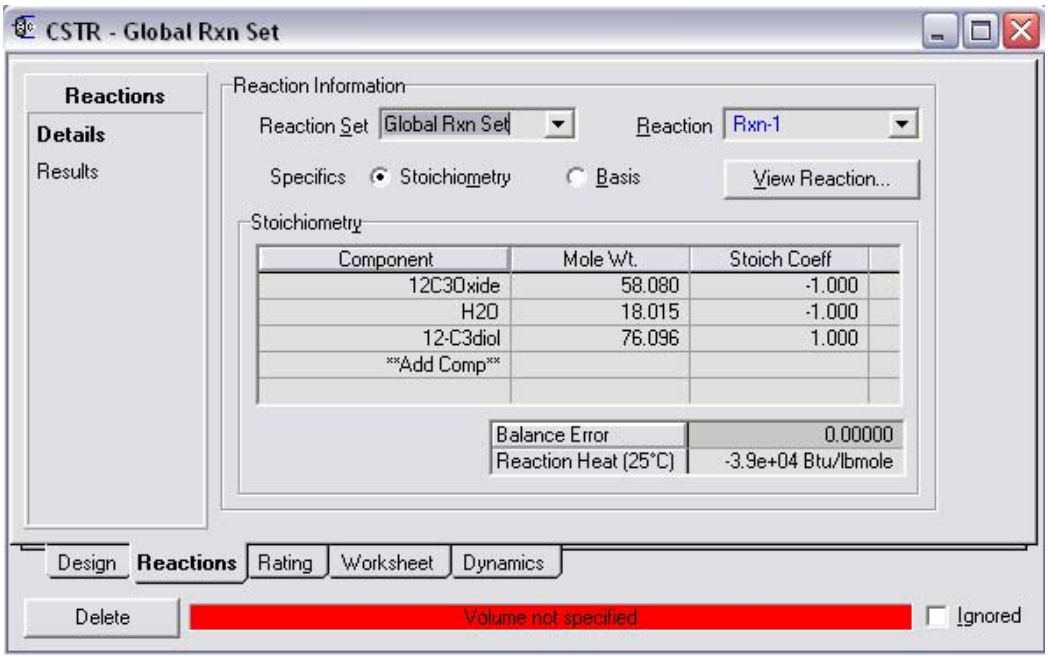


Figure 10-12

4. The next task is to specify the **Vessel Parameters**. In this case, the reactor has a volume of 280 ft^3 and is 85% full.
5. Click the **Dynamics** tab, then select the **Specs** page.
6. In the Model Details group, click in the **Vessel Volume** cell. Type **280** (ft3).
7. In the **Liq Volume Percent** cell, type **85**.

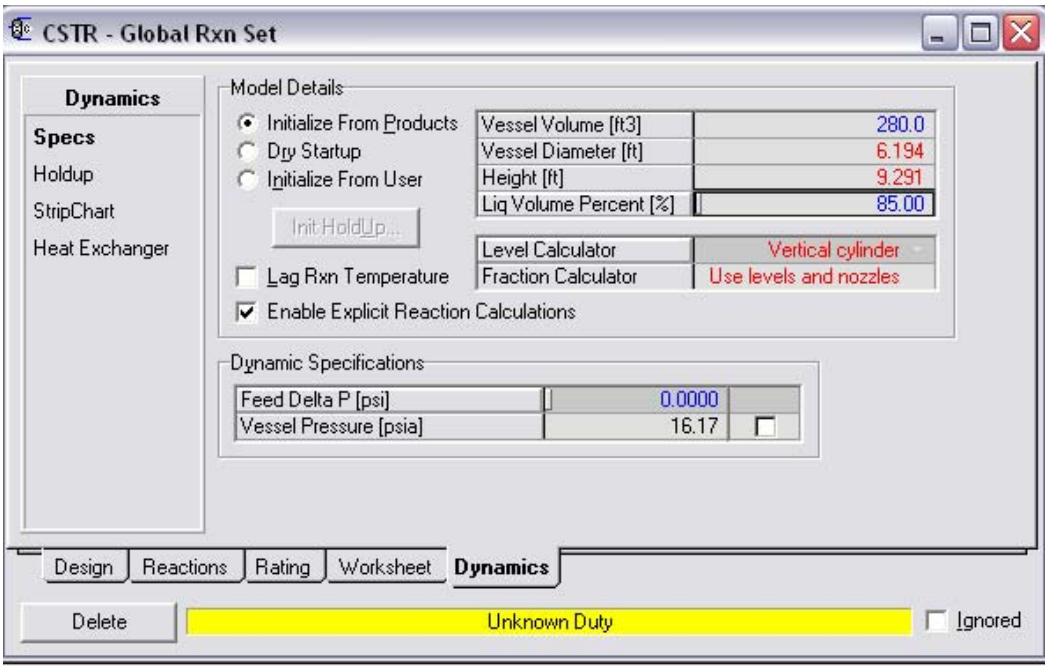


Figure 10-13

8. Click on the **Worksheet** tab. At this point, the reactor product streams and the energy stream coolant are unknown because the reactor has one degree of freedom. At this point, either the outlet stream temperature or the cooling duty can be specified.
9. Initially the reactor is assumed to be operating at isothermal conditions, therefore, the outlet temperature is equivalent to the feed temperature, 75°F. In the CSTR Product column, enter **75** at the **Temperature** cell.

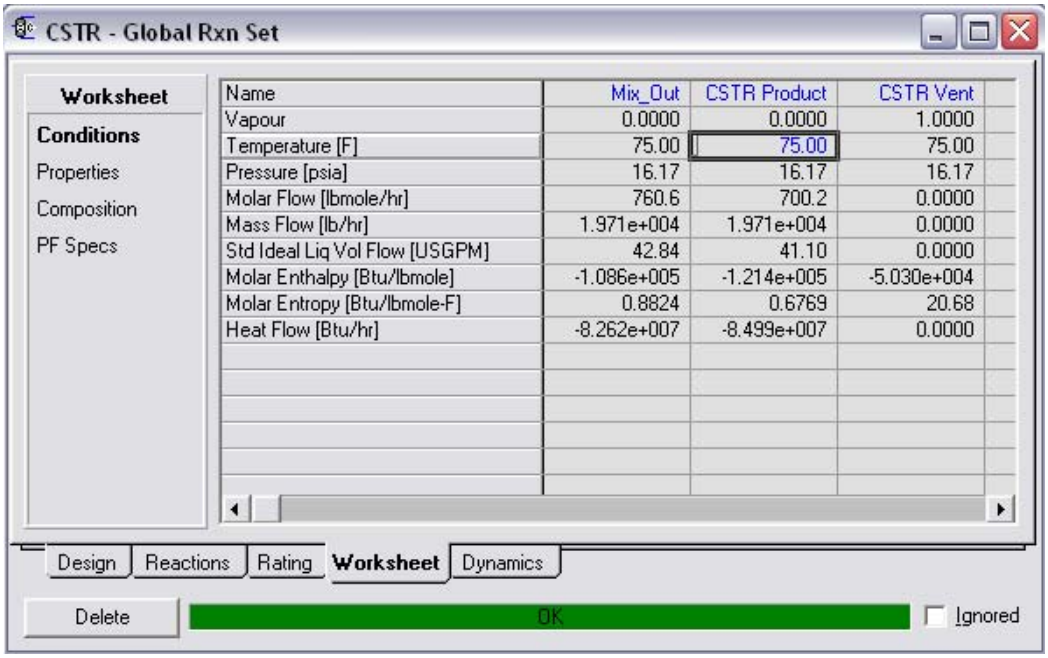


Figure 10-14

10. There is no phase change in the Reactor under isothermal conditions since the flow of the vapor product stream CSTR Vent is zero. In addition, the required cooling duty has been calculated and is represented by the Heat Flow of the Coolant stream. The next step is to examine the Reactor conversion as a function of temperature.
11. Click the **Reactions** tab, then select the **Results** page. The conversion appears in the Reactor Results Summary table.

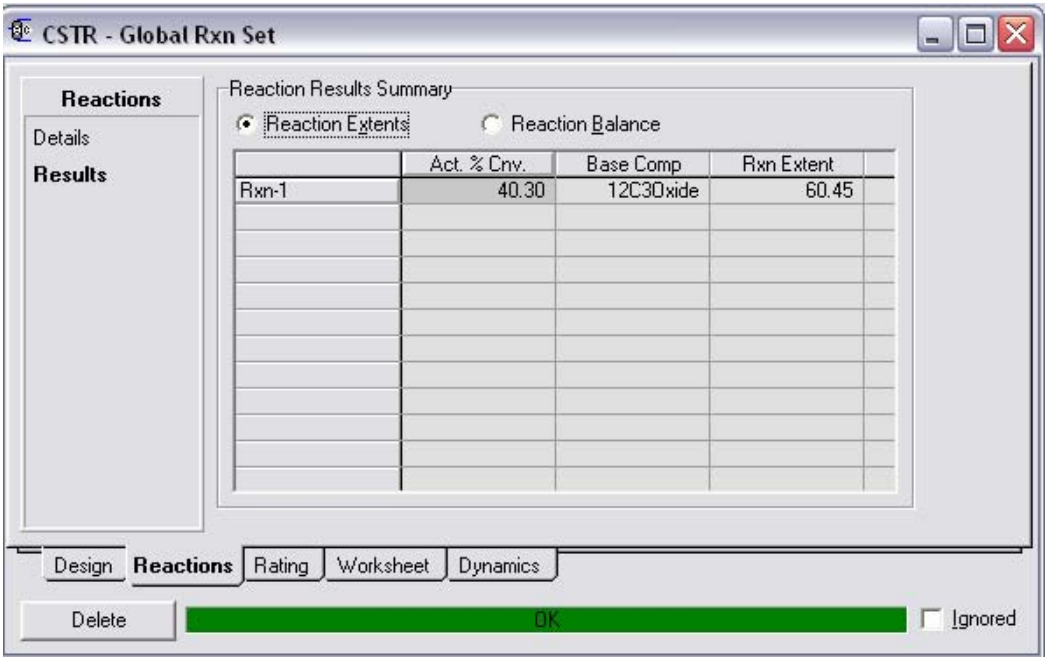


Figure 10-15

12. Under the current conditions, the Actual Percent Conversion (**Act.% Cnv.**) in the Reactor is 40.3%. You need to adjust the reactor temperature until the conversion is in the 85-95% range.

Complete the following:

Reactor Temperature: _____

Actual Percent Conversion: _____

10.9 Save Your Case

1. Go to the **File** menu.
2. Select **Save As**.
3. Give the HYSYS file the name **CSTR** then press the OK button.

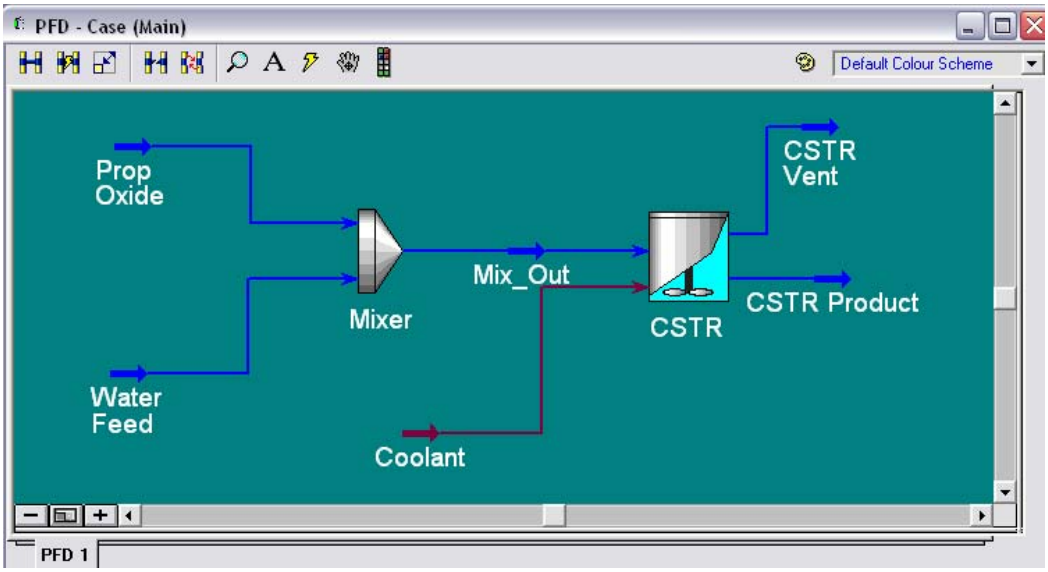


Figure 10-16

10.10 Review and Summary

In this chapter, a flowsheet for the production of propylene glycol is presented. Propylene oxide is combined with water to produce propylene glycol in a continuously-stirred-tank reactor (CSTR).

The propylene oxide and water feed streams are combined in a mixer. The combined stream is fed to a reactor, operating at atmospheric pressure, in which propylene glycol is produced.

Chapter 11
Absorber

Absorber

This chapter introduces the use of Aspen HYSYS to model a continuous gas absorption process in a packed column. The only unit operation contained in the Absorber is the Tray Section, and the only streams are the overhead vapor and bottom liquid products. There are no available specifications for the Absorber, which is the base case for all tower configurations. The conditions and composition of the column feed stream, as well as the operating pressure, define the resulting converged solution. The converged solution includes the conditions and composition of the vapor and liquid product streams.

Learning Outcomes: At the end of this chapter, the user will be able to:

- Operate an absorber operation in HYSYS to model the absorption process
- Determine the column design parameter

Prerequisites: Before beginning this chapter, the users need to know how to:

- Navigate the PFD
- Add Streams in the PFD or the Workbook
- Add and connect Unit Operations

11.1 Problem Statement

CO_2 is absorbed into propylene carbonate in a packed column. The inlet gas stream is 20 mol% CO_2 and 80 mol% methane. The gas stream flows at a rate of 2 m^3/s and the column operates at 60°C and 60.1 atm. The inlet solvent flow is 2000 kmol/h. Use Aspen HYSYS to determine the concentration of CO_2 (mole%) in the exit gas stream, the column height (m) and the column diameter (m).

11.2 Defining the Simulation Basis

2. Enter the following values in the specified fluid package view:

On this page…	Select…
Property Package	Sour PR
Components	CH_4, CO_2, Propylene Carbonate

2. Click the **Enter Simulation Environment** button when you are ready to start building the simulation.

11.3 Adding a Feed Stream

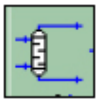
Add a new **Material** stream with the following values.

In this cell…	Enter…
Name	Solvent In
Temperature	60°C
Pressure	60.1 atm
Molar Flow	2000 kgmole/h
Component Mole Fraction	
CO2	0.000
Methane	0.000
C3=Carbonate	1.000

Add another new **Material** stream with the following values.

In this cell…	Enter…
Name	Gases In
Temperature	60°C
Pressure	60.1 atm
Molar Flow	7200 m^3/h
Component Mole Fraction	
CO2	0.200
Methane	0.800
C3=Carbonate	0.000

11.4 Adding an Absorber

1. Double-click on the **Absorber** button on the **Object Palette**, which looks like this, 
2. On the **Connections** page, enter the following information:

In this cell…	Enter…
Name	Absorber
Top Stage Inlet	Solvent In
Bottom Stage Inlet	Gases In
Ovhd Vapour Outlet	Gases Out
Bottom Liquid Outlet	Liquid Out

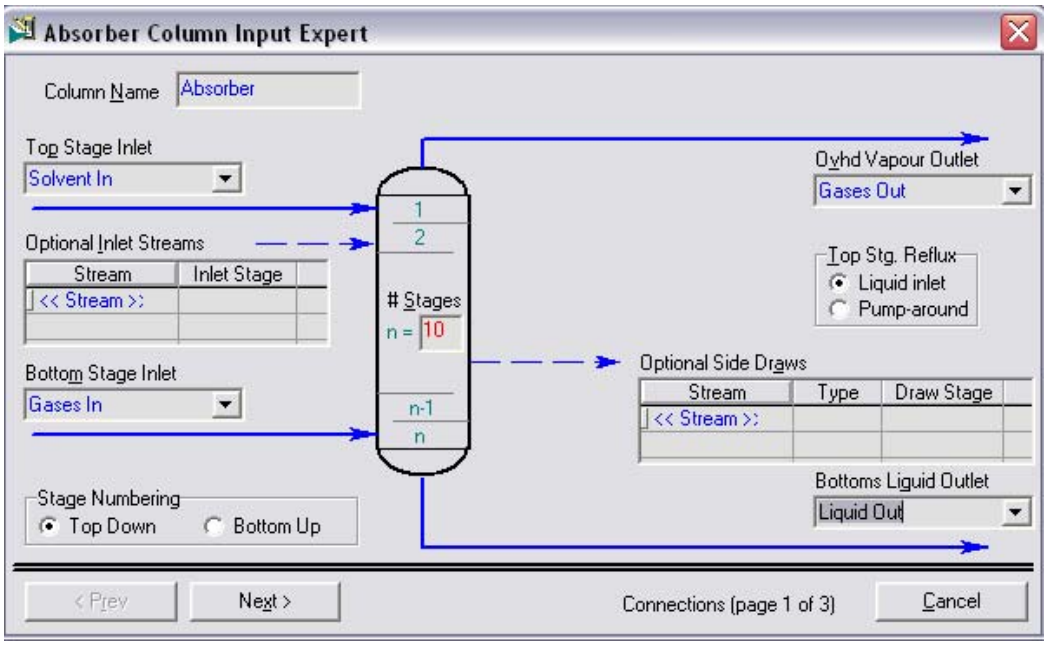


Figure 11-1

3. Click **Next**, and then enter the following information as shown in Figure 11-2.

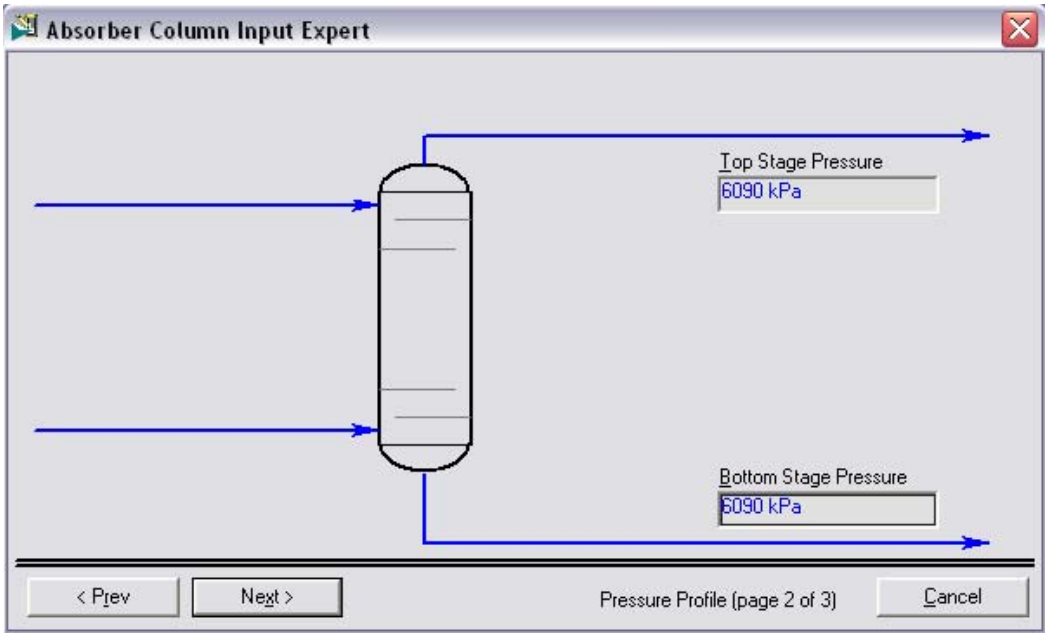


Figure 11-2

4. Click **Next**, and then enter the following information as shown in Figure 11-3. Then, click the **Done…** button.

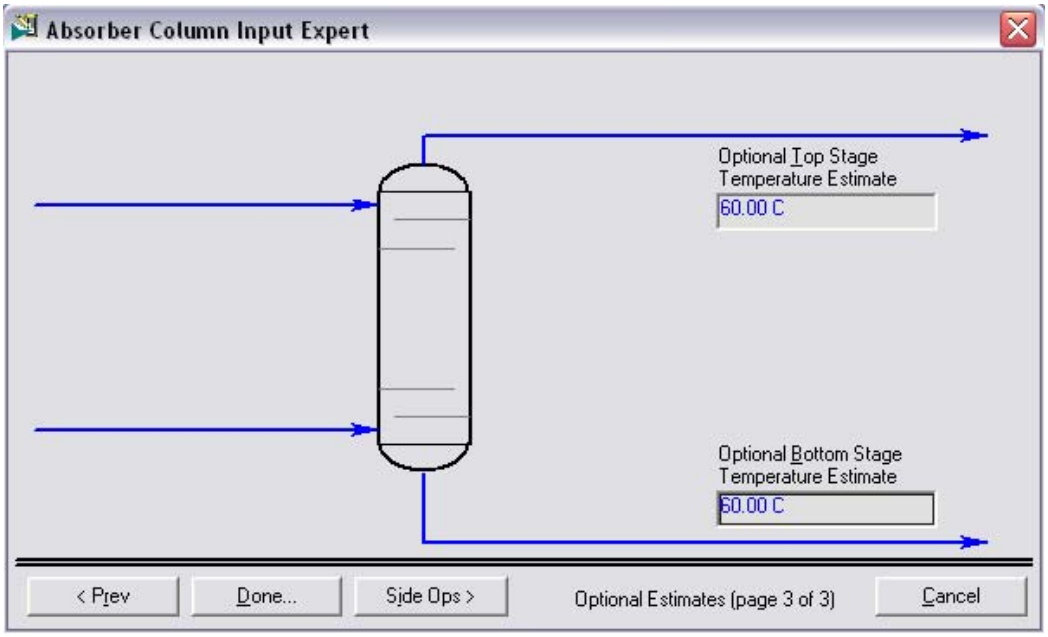


Figure 11-3

5. By clicking on the done button, HYSYS will bring up a window as shown in Figure 11-4.

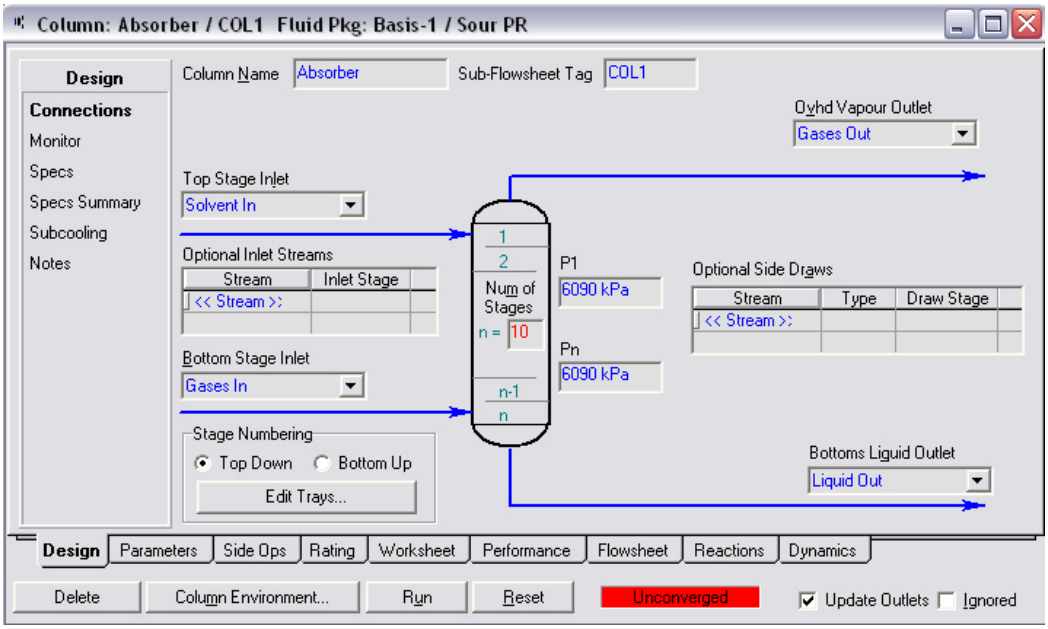


Figure 11-4

11.5 Running the Simulation

When the column window as shown in Figure 11-4 pops up, click on the **Run** button located near the bottom of the window. The red **Unconverged** box should turn to green **Converged** if all the above procedure was followed. However, the results that are obtained at this point do not represent a true model for our gas absorption column because the simulation was run using trays, not packing. Now, let's see how to replace trays with packing.

11.6 Changing Trays to Packing

1. Scroll down and select **Tray Sizing**.
2. Go to the **Tools** menu and select **Utilities**.

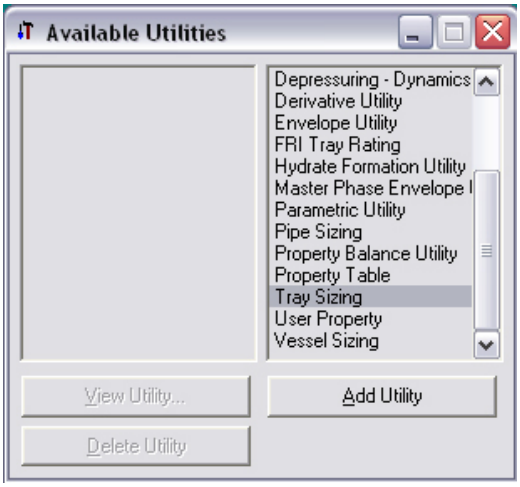


Figure 11-5

3. Click on the **Add Utility** button. A **Tray Sizing** window should pop up. Name the utility as **Packing**.

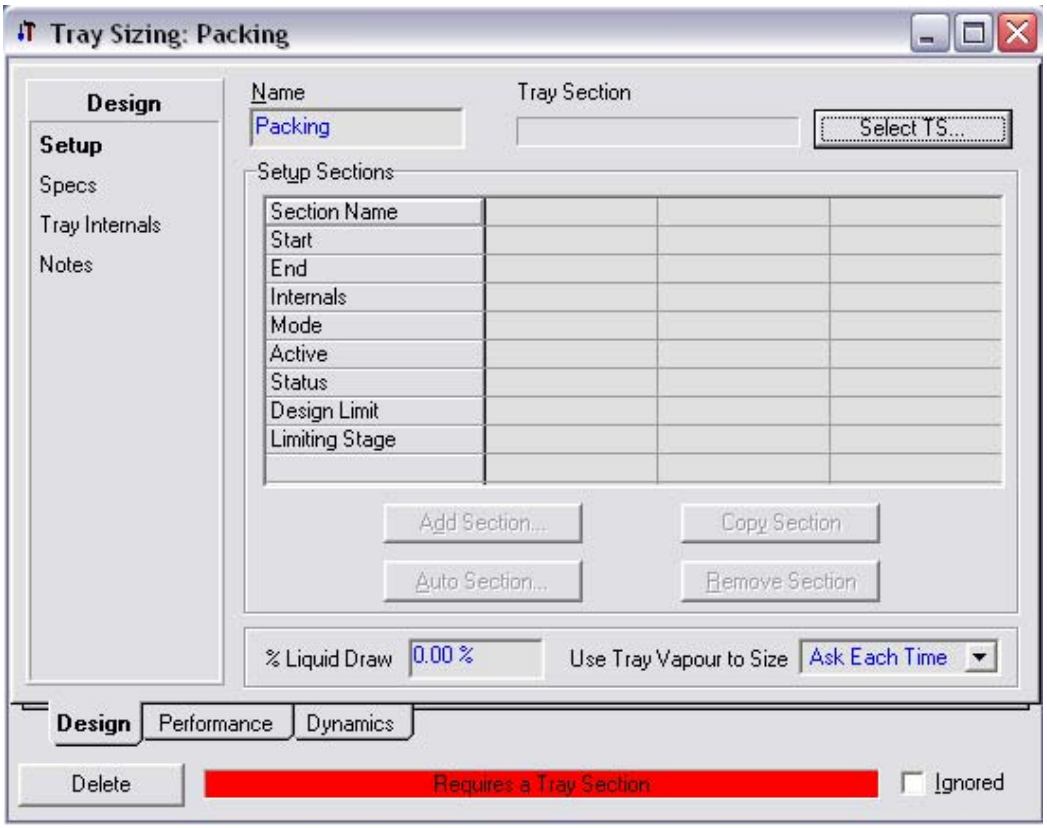


Figure 11-6

4. Click on the **Select TS…** button. Once you select the **Select TS…** button, a window should pop up as shown in Figure 11-7. Make all the selection as shown and then click **OK.**

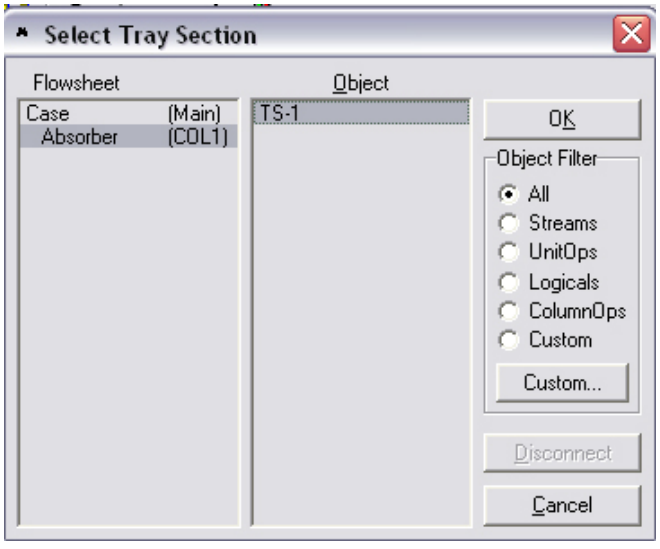


Figure 11-7

5. After selecting the Tray Section, one will return to the **Tray Sizing** window. Click on the button **Auto Section…** For the tray internal type, select **Packed**. A drop down menu box will appear in the window. Scroll the drop down menu box and choose Raschig Rings (Ceramic) 1_4_inch.

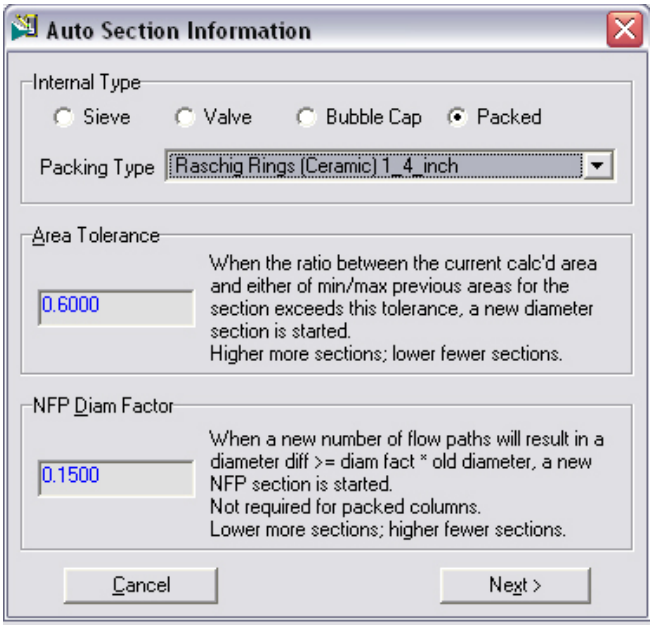


Figure 11-8

6. When the selection is made, click on the **Next >** button. In the next window that appears, click on **Complete AutoSection**.

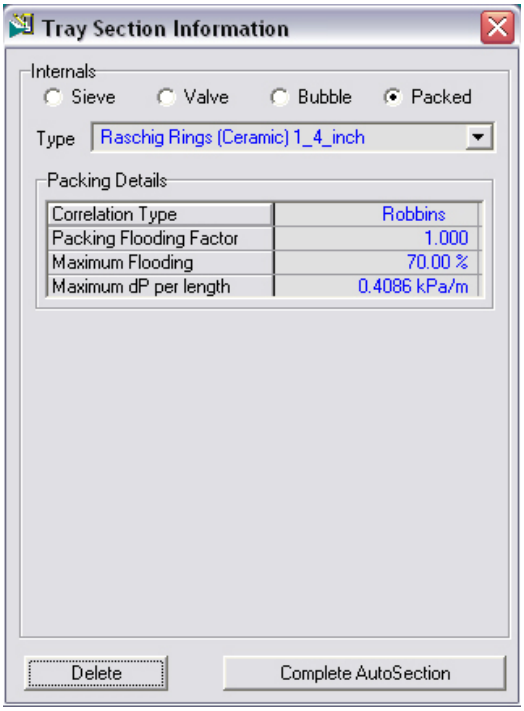


Figure 11-9

7. In the next window that appears, click on **Complete AutoSection**. The **Tray Sizing** window should appear. Now close this window and go to the **PFD** window.
8. Double-click on **Absorber** and run the simulation again.

11.7 Getting the Design Parameters

1. Go to the **Tools** menu and click on **Utilities**.
2. A window names **Available Utilities** will pop up. Select **Packing** and click on **View Utility…** button.
3. On the window that pops-up, click on **Auto Section…** and change the internal type selection to **Packed**. You do not have to select the type of packing again.
4. Click on **Next >** and then on **Complete AutoSection**.
5. Now, click on the **Performance** tab and select **Packed**.
6. In the section results, you can see the diameter and the height of the section.

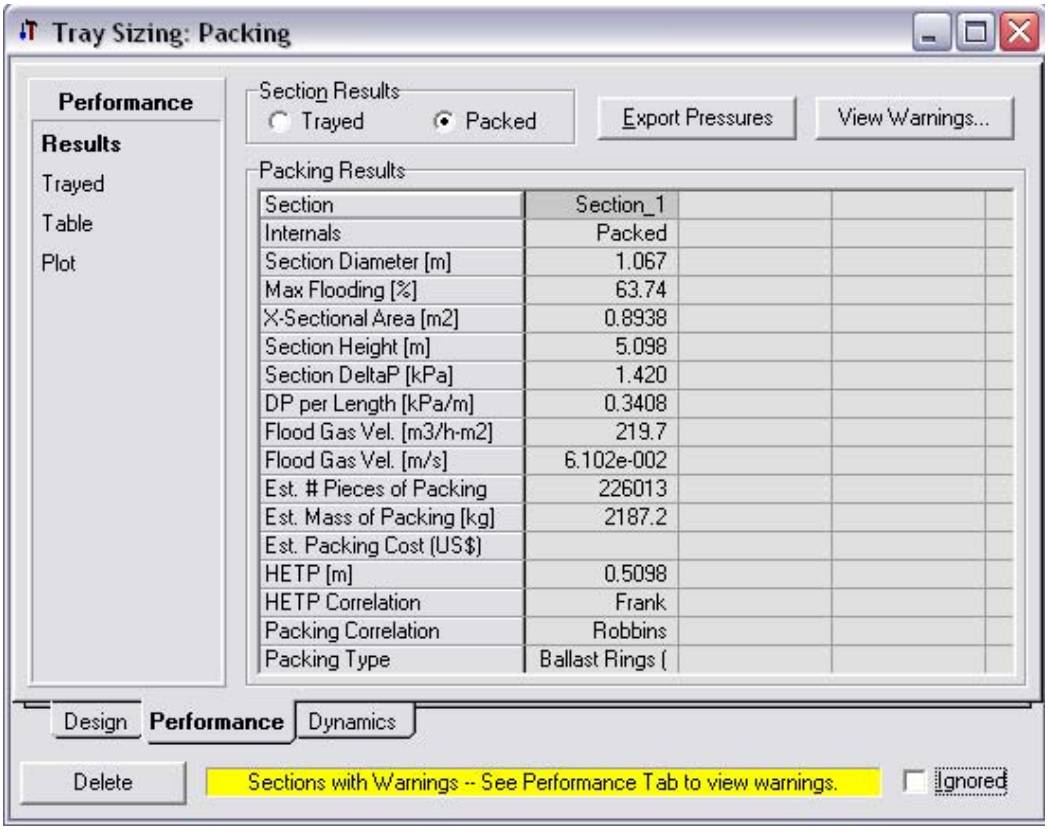


Figure 11-10

7. Now, go back to the PFD window and double-click on the **Gases Out** stream and note the composition of CO_2.

Section Diameter (m): _____

Section Height (m): _____

CO_2 composition: _____

11.8 Save Your Case

1. Go to the **File** menu.
2. Select **Save As**.
3. Give the HYSYS file the name **Absorber** then press the OK button.

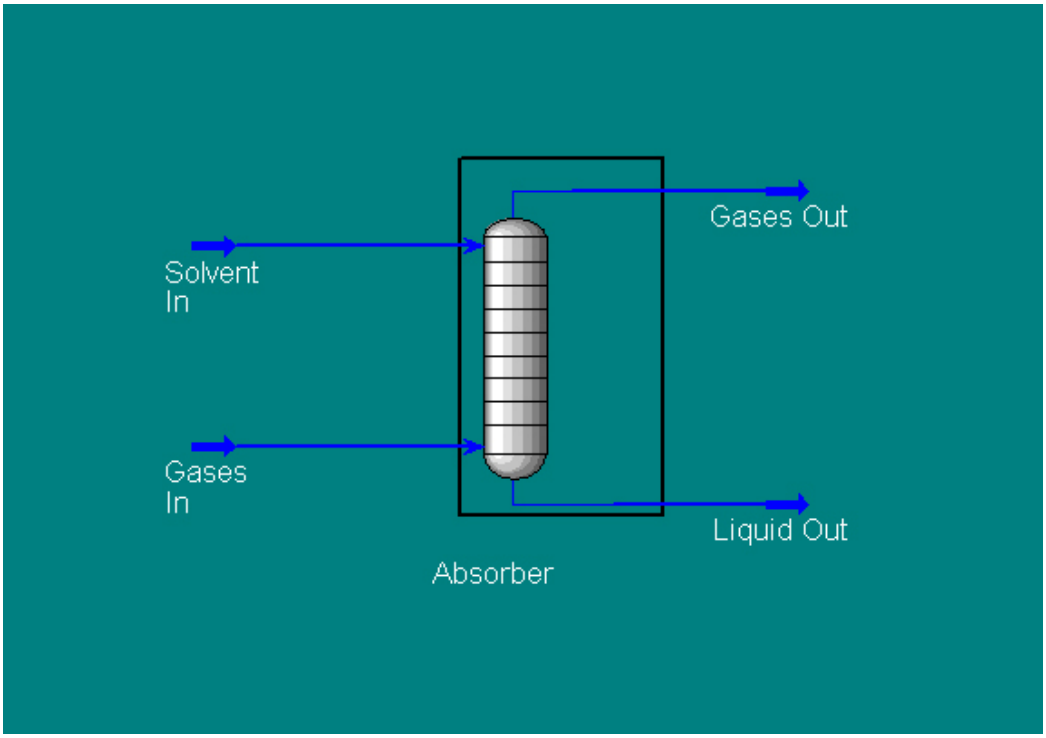


Figure 11-11

11.9 Review and Summary

In the first part of this chapter, we started with a problem to model an absorber that will absorb CO_2 into propylene carbonate in a packed column. In this chapter the user operated an absorber operation in HYSYS to model an absorption process.

At the end of this chapter, the user was asked to use Aspen HYSYS to determine the concentration of CO_2 (mole%) in the exit gas stream, the column height (m) and the column diameter (m).

11.10 Further Study

Change the **Solvent In** flowrate from 2000 kmole/h to 2500 kmol/h. Run the simulation and see how the column dimension and exit concentration of CO_2 have changed.

Section Diameter (m): _____

Section Height (m): _____

CO_2 composition: _____

Chapter 12
Separation Columns

Separation Columns

Recovery of natural-gas liquids (NGL) from natural gas is quite common in natural gas processing. Recovery is usually done to:

- Produce transportable gas (free from heavier hydrocarbons which may condense in the pipeline).
- Meet a sales gas specification.
- Maximize liquid recovery (when liquid products are more valuable than gas).

HYSYS can model a wide range of different column configurations. In this simulation, an NGL Plant will be constructed, consisting of three columns:

- De-Methanizer (operated and modelled as a Reboiled Absorber column)
- De-Ethanizer (Distillation column)
- De-Propanizer (Distillation column)

Learning Outcomes: At the end of this chapter, the user will be able to:

- Add columns using the Input Experts.
- Add extra specifications to columns.

Prerequisites: Before beginning this chapter, the users need to know how to:

- Navigate the PFD
- Add Streams in the PFD or the Workbook
- Add and connect Unit Operations

12.10 Process Overview

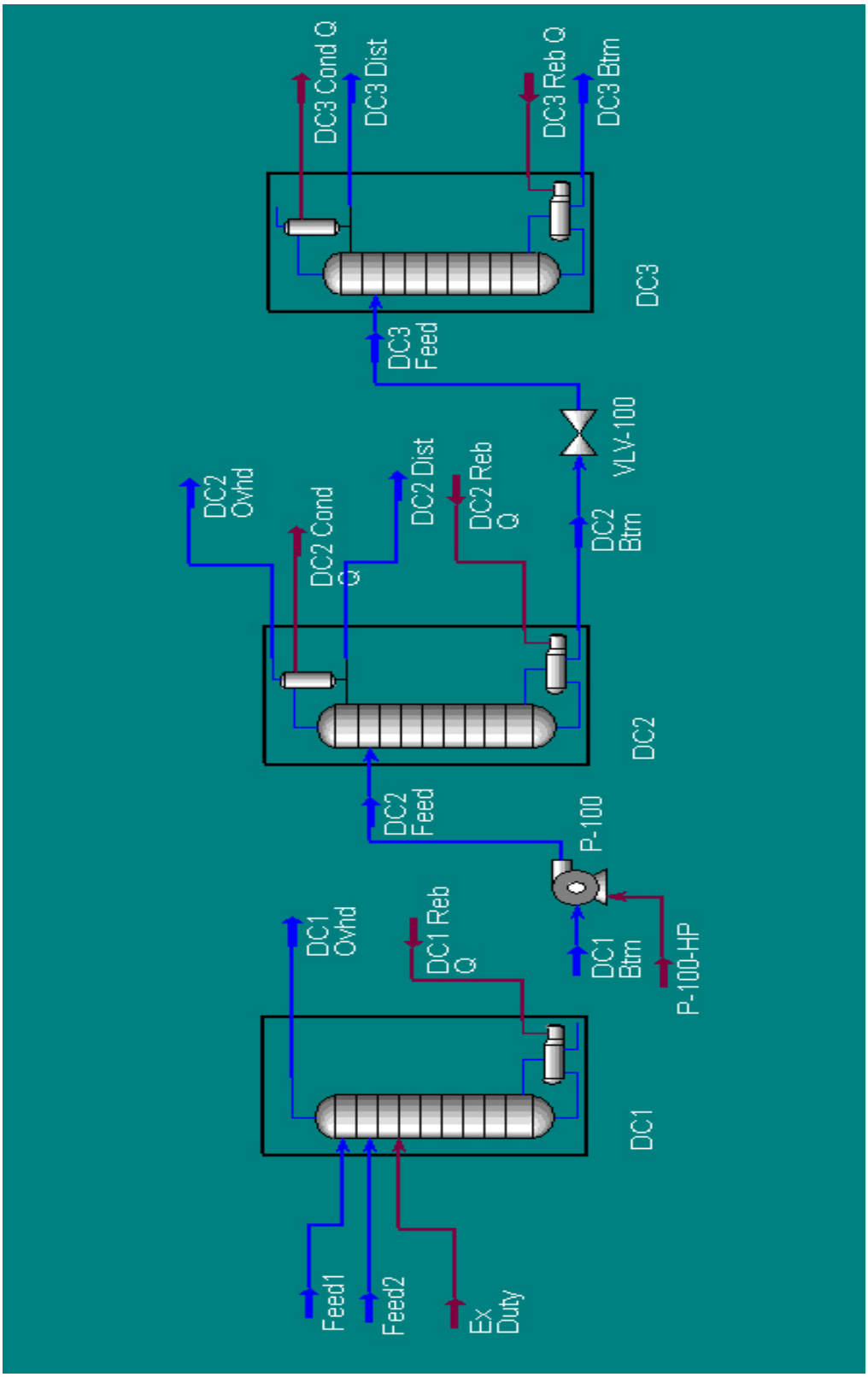


Figure 12-1

12.10 Column Overviews

DC1: De-Methanizer

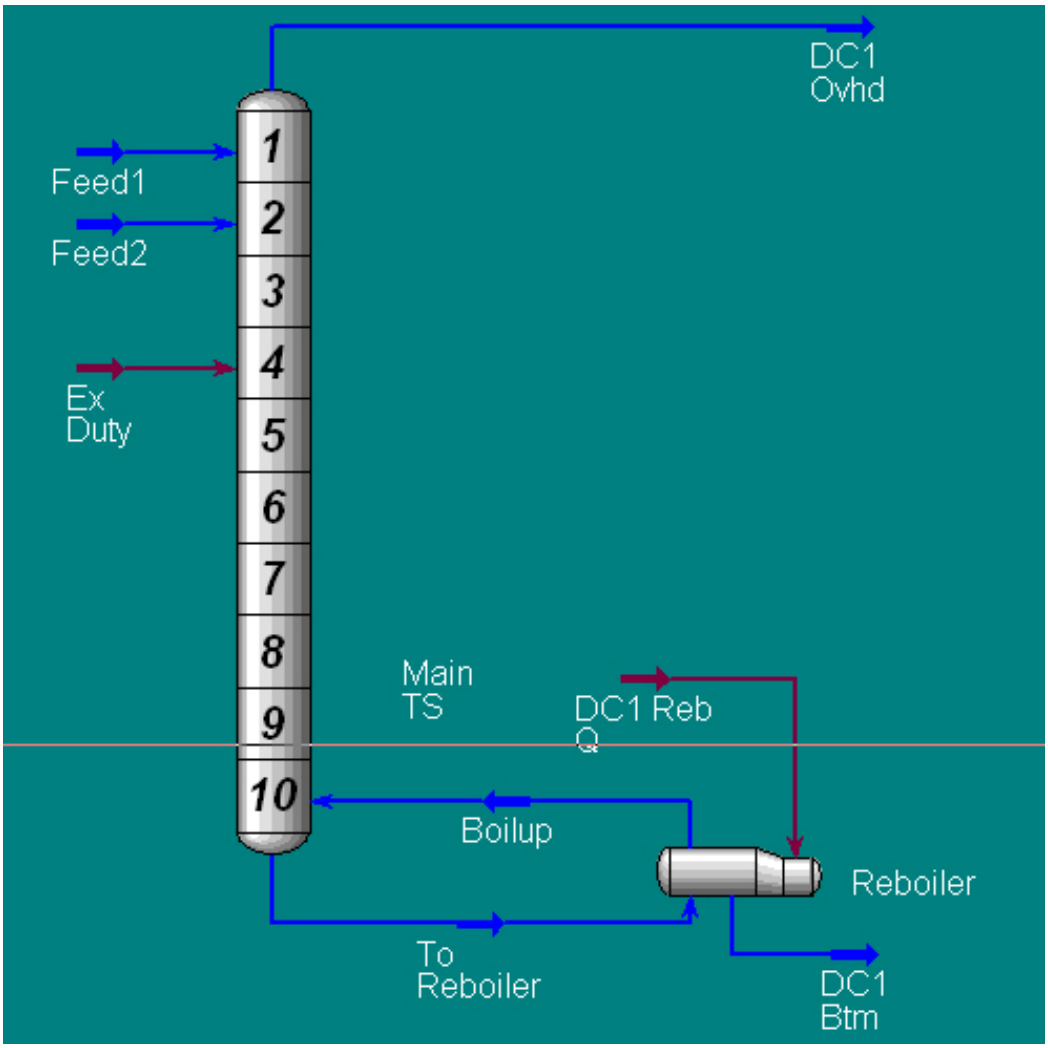


Figure 12-2

DC2: De-Ethanizer

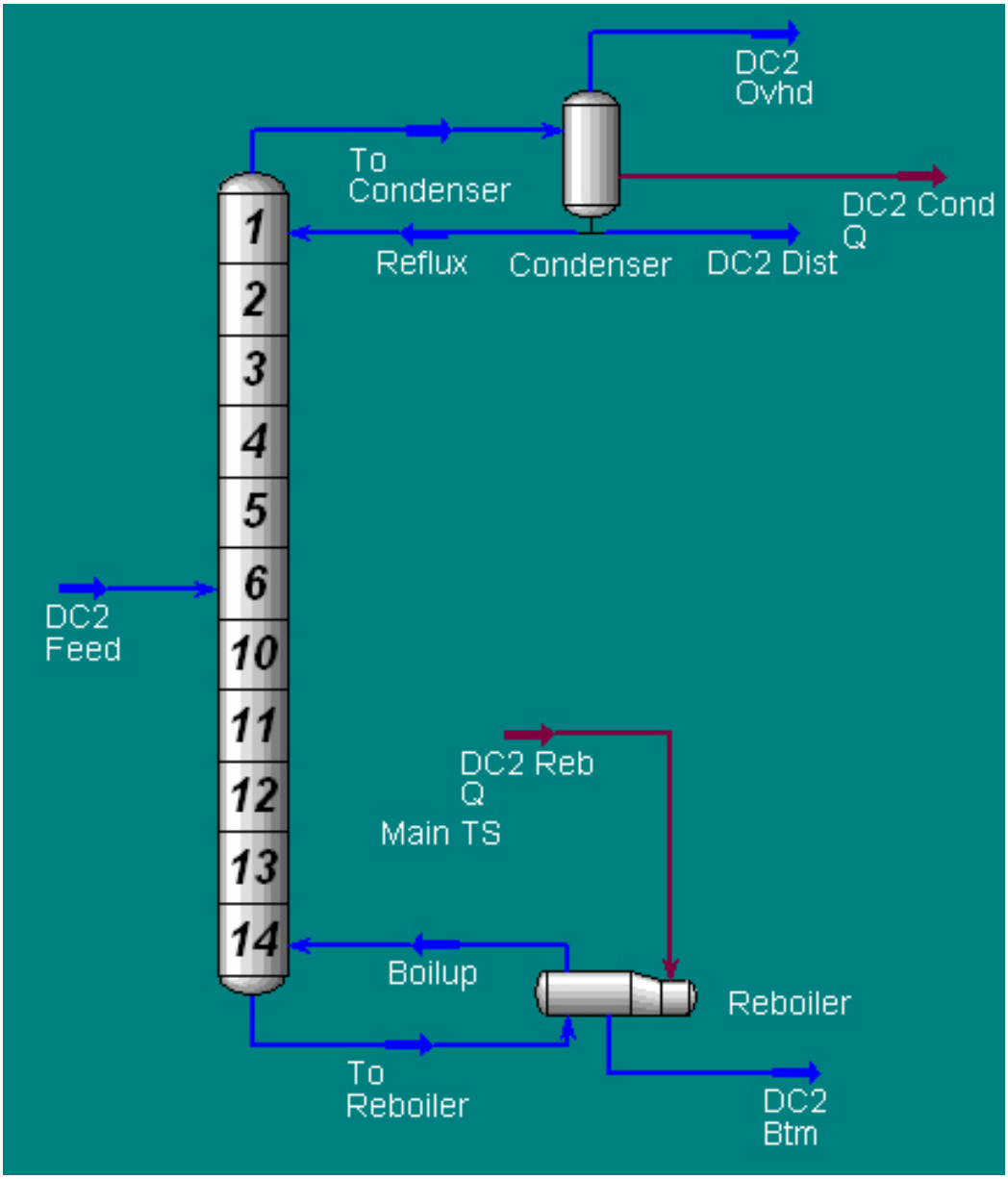


Figure 12-3

DC3: De-Propanizer

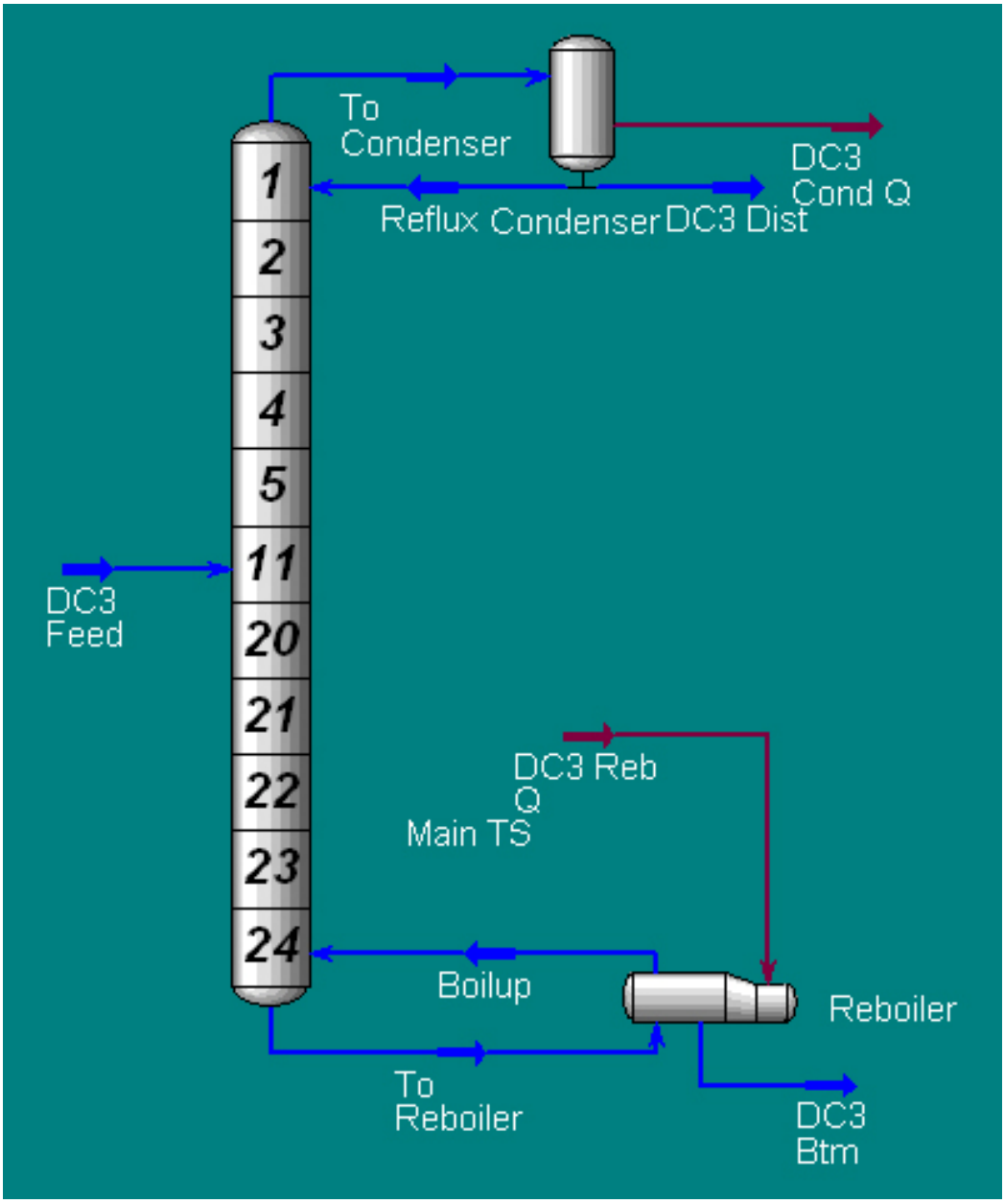


Figure 12-4

12.10 Defining the Simulation Basis

1. Start a new case.
2. Select the **Peng Robinson** EOS.
3. Add the components: N_2, CO_2, C_1 - C_8.
4. Enter the **Simulation Environment**.

12.4 Adding the Feed Streams

1. Add a **Material Stream** with the following data:

In this cell…	Enter…
Name	Feed1
Temperature	-95°C (-140°F)
Pressure	2275 kPa (330 psia)
Flowrate	1620 kgmole/h (3575 lbmole/hr)
Component	Mole Fraction
N_2	0.0025
CO_2	0.0048
C_1	0.7041
C_2	0.1921
C_3	0.0706
i-C_4	0.0112
n-C_4	0.0085
i-C_5	0.0036
n-C_5	0.0020
C_6	0.0003
C_7	0.0002
C_8	0.0001

2. Add another **Material Stream** with the following data:

In this cell…	Enter…
Name	Feed2
Temperature	-85°C (-120°F)
Pressure	2290 kPa (332 psia)
Flowrate	215 kgmole/h (475 lbmole/hr)
Component	Mole Fraction
N_2	0.0057
CO_2	0.0029
C_1	0.7227
C_2	0.1176
C_3	0.0750
i-C_4	0.0204
n-C_4	0.0197
i-C_5	0.0147
n-C_5	0.0102
C_6	0.0037
C_7	0.0047
C_8	0.0027

12.5 Adding De-Methanizer

The De-Methanizer is modelled as a reboiled absorber operation, with two feed streams and an energy stream feed, which represents a side heater on the column.

1. Add an **Energy** stream with the following values:

In this cell…	Enter…
Name	Ex Duty
Energy Flow	2.1e+06 kJ/h (2.0e+06 Btu/hr)

2. Double-click on the **Reboiled Absorber** icon on the Object Palette. The first Input Expert view appears.


Reboiled Absorber Column icon

3. Complete the view as shown below:

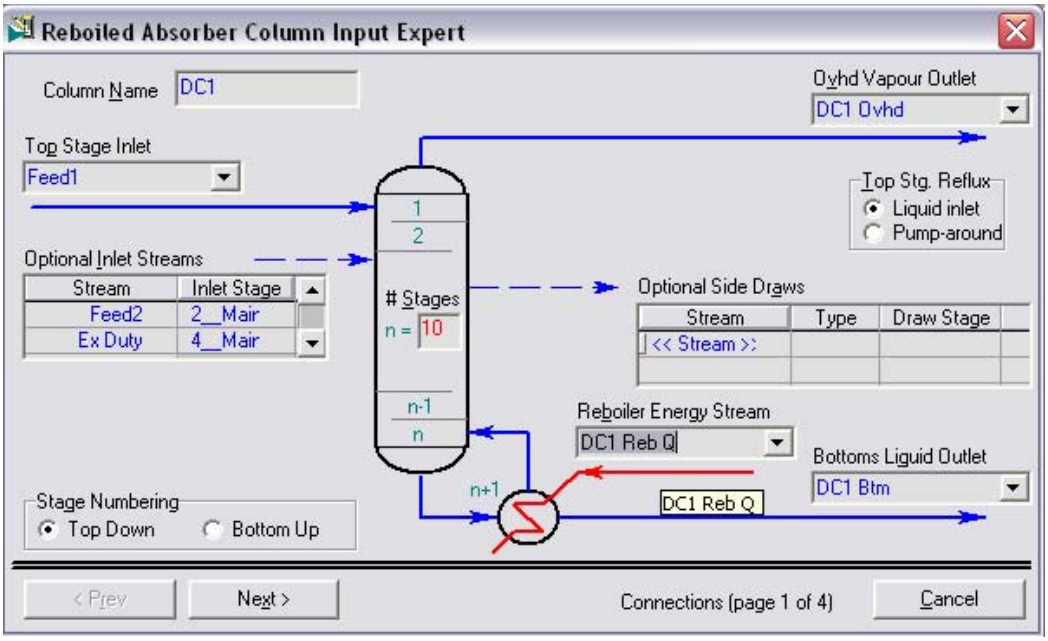


Figure 12-5

4. Click the **Next** button to proceed to the next page.
5. Supply the following information to the Pressure Estimates page. If you are using field units, the values will be **330 psia** and **335 psia**, for the Top Stage Pressure and Reboiler Pressure, respectively.

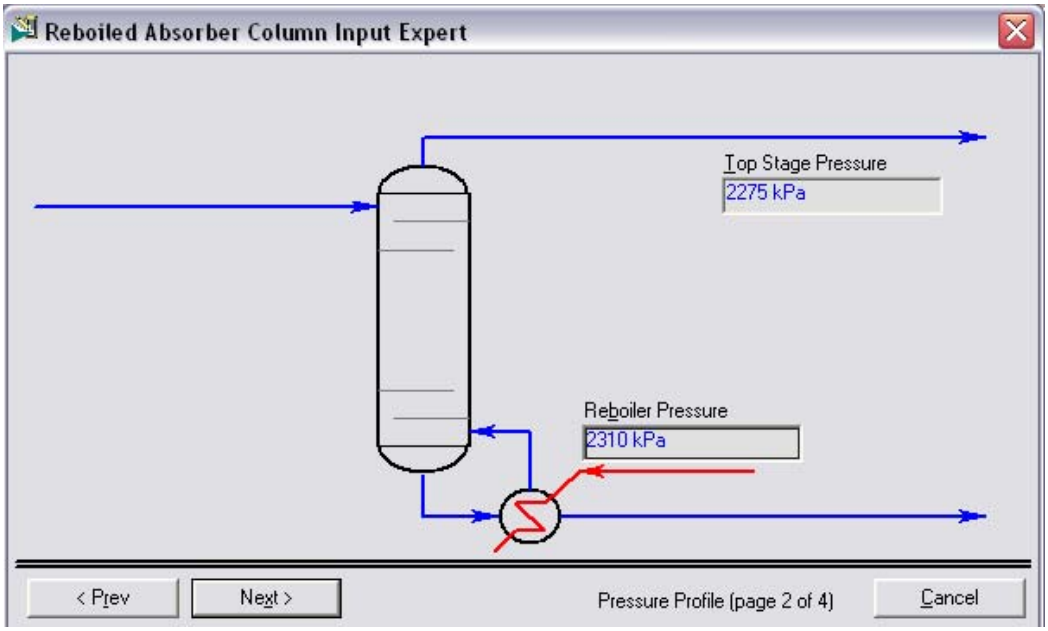


Figure 12-6

6. Click the **Next** button to proceed to the next page.
7. Enter the temperature estimates shown below. In field units, the top stage temperature estimate will be **-125°F**, and the reboiler temperature estimate will be **80°F**.

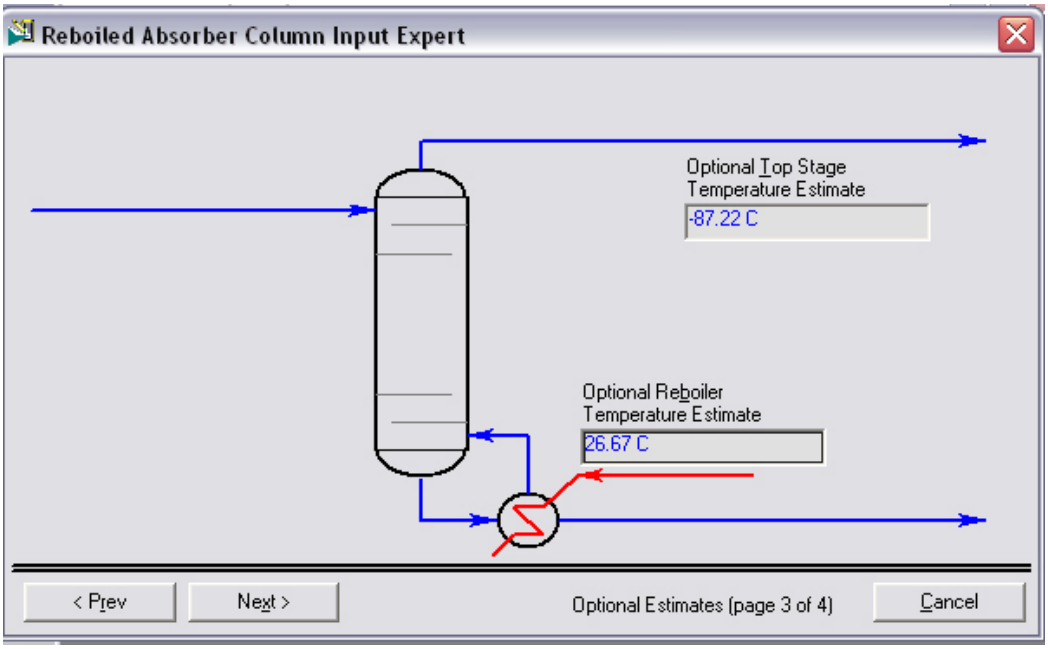


Figure 12-7

8. Click the **Next** button to continue.
9. For this case, no information is supplied on the last page of the Input Expert, so click the **Done** button.

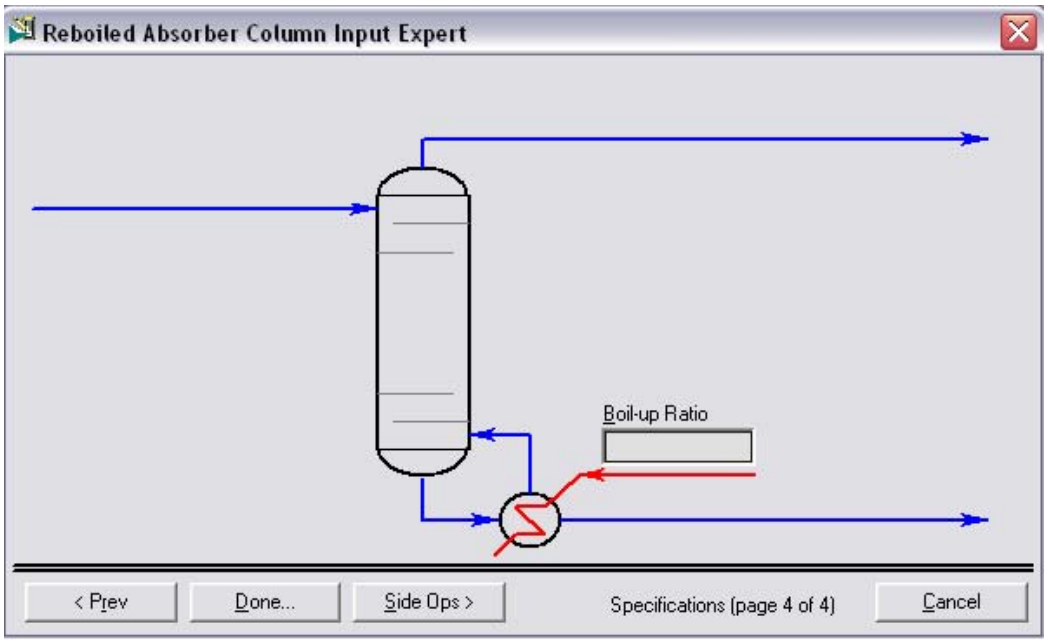


Figure 12-8

When you click the **Done** button, HYSYS will open the Column property view. Access the **Monitor** page on the **Design** tab.

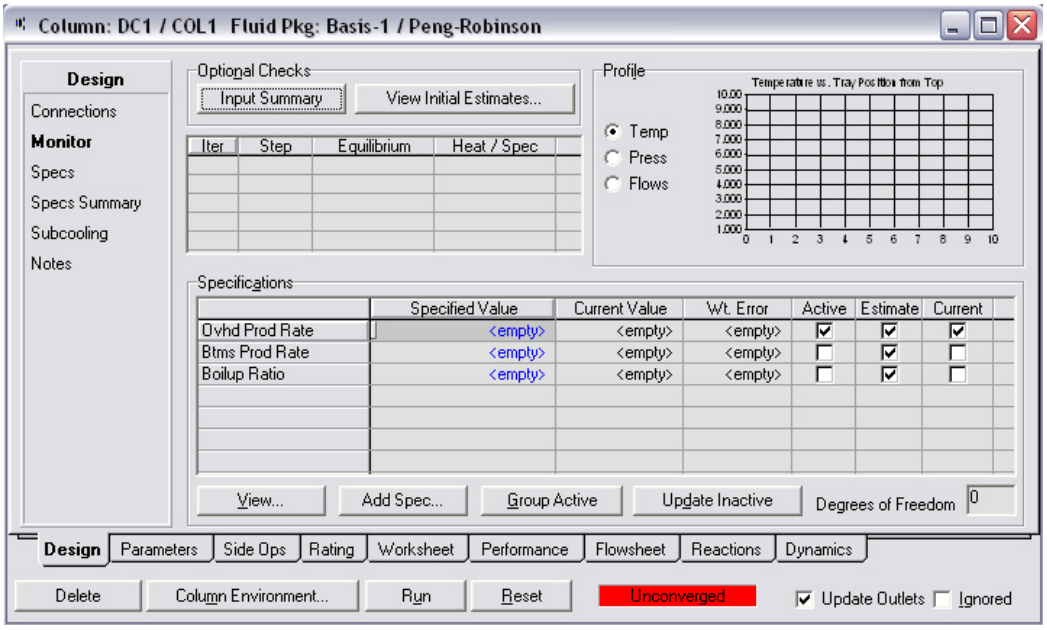


Figure 12-9

Before you converge the column, make sure that the specifications are as shown above. You will have to enter the value for the Ovhd Prod Rate specification. The specified value is **1338 kgmole/h** (2950 lbmole/hr). Once this value is entered, the column will start running and should converge.

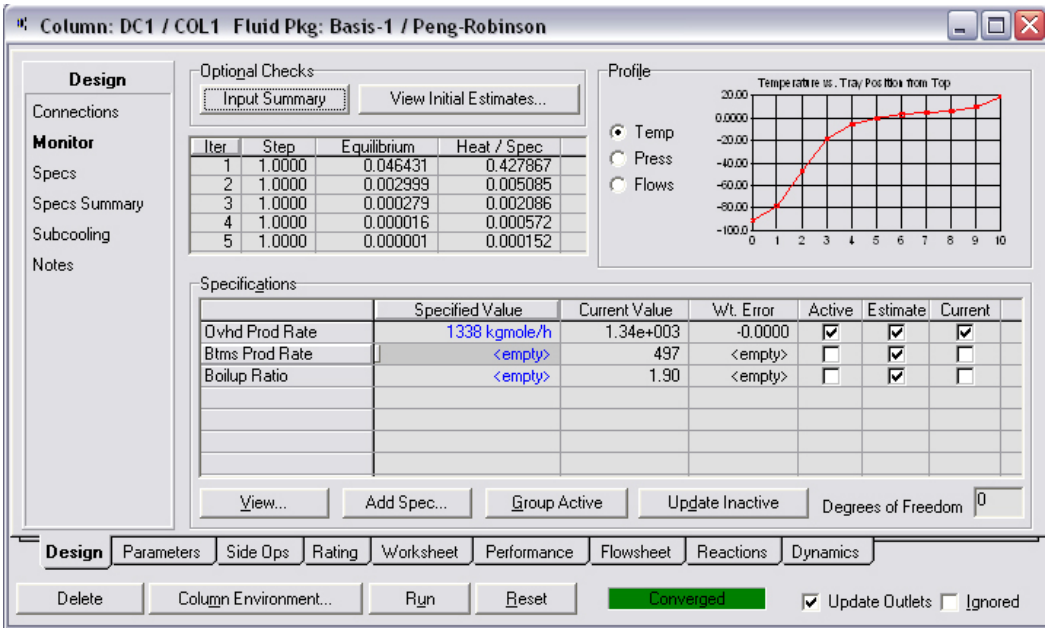


Figure 12-10

What is the mole fraction of Methane in DC1 Ovhd? _____

Although the column is converged, it is not always practical to have flow rate specifications. These specifications can result in columns which cannot be converged or that produce product streams with undesirable properties if the column feed conditions change.

An alternative approach is to specify either component fractions or component recoveries for the column product streams.

1. Go to the **Specs** page on the **Design** tab of the Column property view.

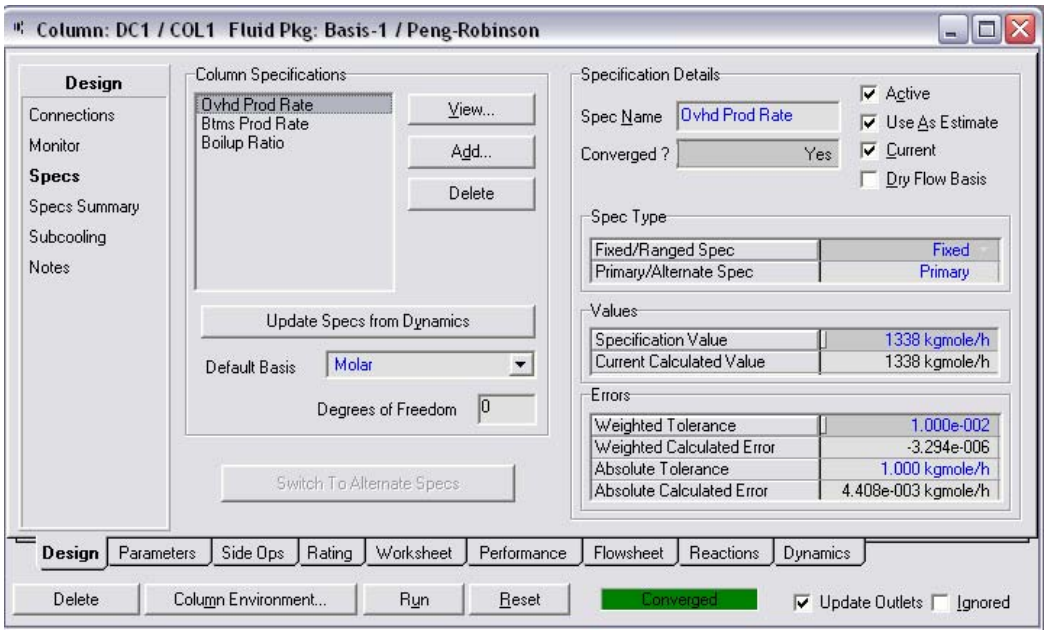


Figure 12-11

2. Click the **Add** button in the Column Specifications group to create a new specification.
3. Select **Column Component Fraction** from the list that appears.

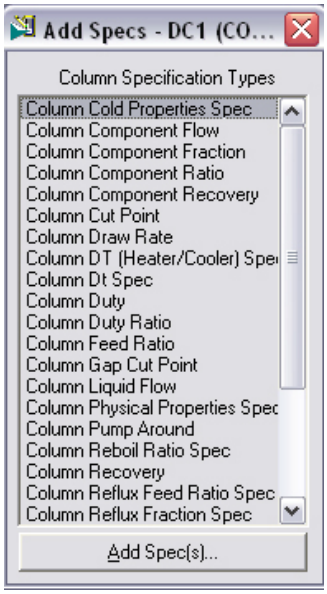


Figure 12-12

4. Click the **Add Spec(s)** button.
5. Complete the spec as shown in the following figure.

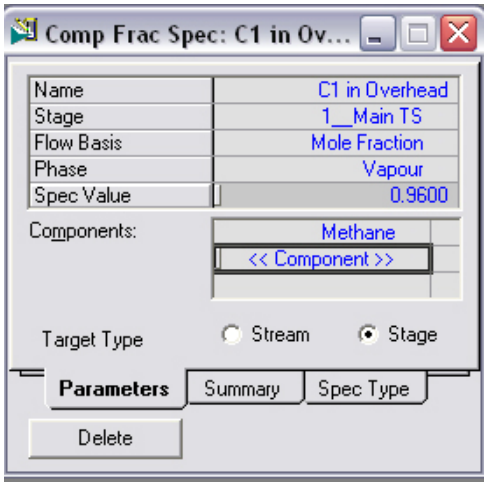


Figure 12-13

6. When you are done, close the view.

The Monitor page of the Column property view shows 0 Degrees of Freedom even though you have just added another specification. This is due to the fact that the specification was added as an estimate, not as an active specification.

7. Go to the **Monitor** page. Deactivate the **Ovhd Prod Rate** as an active specification and activate the **Comp Fraction** specification which you created.

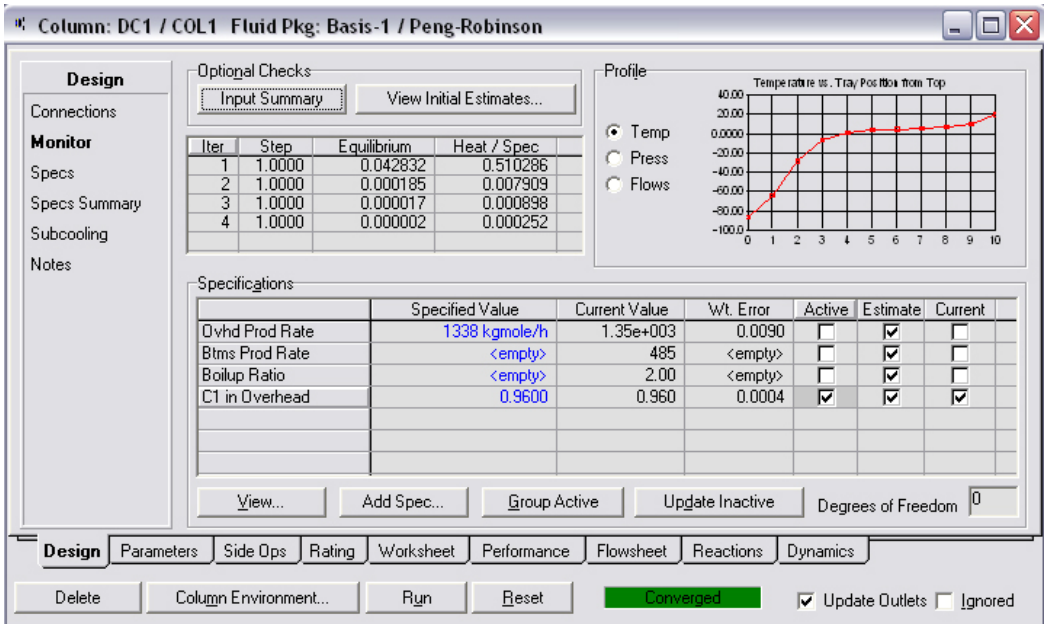


Figure 12-14

What is the flowrate of the overhead product, DC1 Ovhd? _____

Once the column has converged, you can view the results on the **Performance** tab.

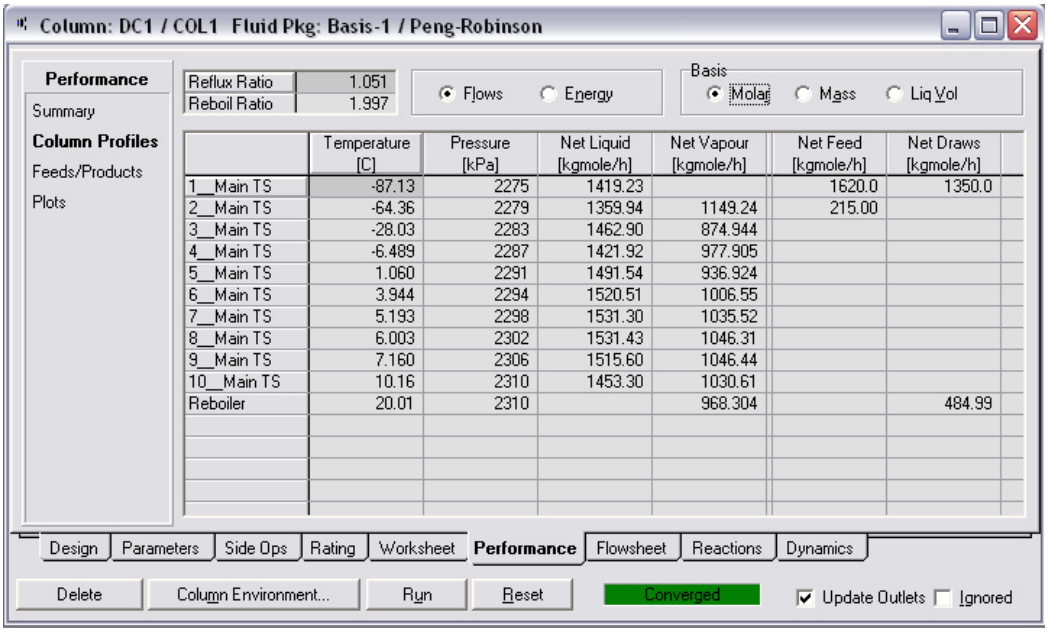


Figure 12-15

12.6 Adding a Pump

The pump is used to move the De-Methanizer bottom product to the De-Ethanizer.

Install a pump and enter the following information:

In this cell…	Enter…
Connections	
Inlet	DC1 Btm
Outlet	DC2 Feed
Energy	P-100-HP
Worksheet	
DC2 Feed Pressure	2790 kPa (405 psia)

12.7 De-Ethanizer

The De-Ethanizer column is modeled as a distillation column, with 16 stages, 14 trays in the column, plus the reboiler and condenser. It operates at a pressure of 2760 kPa (400 psia). The objective of this column is to produce a bottom product that has a ratio of ethane to propane of 0.01.

1. Double-click on the **Distillation Column** button on the Object Palette and enter the following information.

Distillation Column icon

In this cell…	Enter…
Connections	
Name	DC2
No. of Stages	14
Feed Stream/Stage	DC2 Feed/6
Condenser Type	Partial
Overhead Vapour Product	DC2 Ovhd
Overhead Liquid Product	DC2 Dist
Bottom Product	DC2 Btm
Reboiler Duty	DC2 Reb Q
Condenser Duty	DC2 Cond Q
Pressures	
Condenser	2725 kPa (395 psia)
Condenser Delta P	35 kPa (5 psi)
Reboiler	2792 kPa (405 psia)
Temperature Estimates	
Condenser	-4°C (25°F)
Reboiler	95°C (200°F)
Specifications	
Overhead Vapour Rate	320 kgmole/h (700 lbmole/hr)
Distillate Rate	0 kgmole/h
Reflux Ratio	2.5 (Molar)

2. Click the **Run** button to run the column.

What is the flowrate of C_2 and C_3 in DC2 Btms?

*C_2*_____, *C_3*_____, *Ratio of C_2/C_3*_____

3. On the **Specs** page, click the **Add** button to create a new specification.
4. Select **Column Component Ratio** as the specification type and provide the following information:

In this cell…	Enter…
Name	C2/C3
Stage	Reboiler
Flow Basis	Mole Fraction
Phase	Liquid
Spec Value	0.01
Numerator	Ethane
Denominator	Propane

5. On the **Monitor** tab, deactivate the **Ovhd Vap Rate** specification and activate the **C_2/C_3** specification which you created.

What is the flowrate of DC2 Ovhd? _____

12.8 Adding a Valve

A valve is required to reduce the pressure of the stream DC2 Btm before it enters the final column, the De-Propanizer.

Add a Valve operation and provide the following information:

In this cell…	Enter…
Connections	
Feed Stream	DC2 Btm
Product Stream	DC3 Feed
Worksheet	
DC3 Feed Pressure	1690 kPa (245 psia)

12.9 De-Propanizer

The De-Propanizer column is represented by a distillation column consisting of 25 stages, 24 trays in the column plus the reboiler. (Note that a total condenser does not count as a stage). It operates at 1620 kPa (235 psia). There are two process objectives for this column. One is to produce an overhead product that contains no more than 1.50 mole percent of i-C_4 and n-C_4 and the second is that the concentration of propane in the bottom product should be less than 2.0 mole percent.

1. Add a distillation column and provide the following information:

In this cell…	Enter…
Connections	
Name	DC3
No. of Stages	24
Feed Stream/Stage	DC3 Feed/11
Condenser Type	Total
Overhead Liquid Product	DC3 Dist
Bottom Product	DC3 Btm
Reboiler Duty	DC3 Reb Q
Condenser Duty	DC3 Cond Q
Pressures	
Condenser	1585 kPa (230 psia)
Condenser Delta P	35 kPa (5 psi)
Reboiler	1655 kPa 240 psia)
Temperature Estimates	
Condenser	38^{o}C (100^{o}F)
Reboiler	120^{o}C (250^{o}F)
Specifications	
Distillate Rate	100 kgmole/h (240 lbmole/hr)
Reflux Ratio	1.0 (Molar)

2. Run the column.

What is the mole fraction of C_3 in the overhead and bottoms products?

_____ *and* _____

3. Create two new Component Fraction specifications for the column.

In this cell…	Enter…
i-C4 and n-C4 in Distillate	
Name	iC4 and nC4
Stage	Condenser
Flow Basis	Mole Fraction
Phase	Liquid
Spec Value	0.015
Components	i-C4 and n-C4
C3 in Reboiler Liquid	
Name	C3
Stage	Reboiler
Flow Basis	Mole Fraction
Phase	Liquid
Spec Value	0.02
Component	C3

4. Deactivate the **Distillate Rate** and **Reflux Ratio** specifications.
5. Activate the **iC_4, and nC_4**, and **C_3** specifications which you created.

12.10 Save Your Case

1. Go to the **File** menu.
2. Select **Save As**.
3. Give the HYSYS file the name **Separation Columns** then press the OK button.

Chapter 13
Examples

Examples

This chapter will test the user ability and understanding in solving simple process engineering problems using HYSYS. HYSYS is an interactive process engineering and simulation program. It is powerful program that you can use to solve all kinds of process related problems. However, since you have to provide various conditions and choices in order to solve a problem, you cannot use it effectively unless you have good knowledge about the process and solution procedures.

Learning Outcomes: At the end of this chapter, the user will be able to:

- Manipulate the HYSYS interface and produce the process PFD from the text description.
- Explore process engineering options in process modeling.
- Assess the effect of selected thermodynamics property package on simulation results
- Extract a selection of physical properties from HYSYS

Prerequisites: Before beginning this chapter, the users should finish all the previous chapters.

13.1 Example 1: Process Involving Reaction and Separation

Toluene is produced from n-heptane by dehydrogenation over a Cr_2O_3 catalyst:

$$CH_3CH_2CH_2CH_2CH_2CH_2CH_3 \rightarrow C_6H_5CH_3 + 4H_2$$

The toluene production process is started by heating n-heptane from 65 to 800 ^oF in a heater. It is fed to a catalytic reactor, which operates isothermally and converts 15 mol% of the n-heptane to toluene. Its effluent is cooled to 65 ^oF and fed to a separator (flash). Assuming that all of the units operated at atmospheric pressure, determine the species flow rates in every stream.

Solution

1. Start HYSYS and File/New/Case.
2. *Simulation Basis Manager* will pop up. Click **Add**. *Fluid Package* window will be opened. Choose **Peng Robinson** as Base Property Package.
3. Open **Component** page of *Fluid Package* window and add components (toluene, *n*-heptane, and hydrogen) and close the *Fluid Package.*
4. Click **Enter Simulation Environment** at the bottom of *Simulation Basis Manager*.
5. Click **Heater** in the *Object Palette* and click it on *Process Flow Diagram (PFD)*. Click General Reactor, three different reactors will pop up, click **conversion** reactor and click it on *PFD*. Do the same for the **Cooler** and **Separator**.
6. Name inlets and outlets of all process units as shown in *PFD* diagram on the Figure 13.1.
7. You will notice that the reactor is colored red with the error message, "Need a reaction set." Now we need to input what the reaction is. Click Flowsheet/Reaction Package. Add Global Rxn Set. Then, click Add Rxn at the lower right side of the window and choose Conversion. Add three components (n-Heptane, Toluene, Hydrogen) and Stoich Coeff (-1, 1, 4). Click Basis page, and type 15 for Co (this is the conversion). Close windows until you see *PFD*.
8. Double click reactor. Choose Global Rxn Set as Reaction set and close the window.
9. Now, open worksheet, and type in all the known conditions for the streams. Note that only blue colored fonts are the values that you specified. If you more information than the degree of freedom allows, it will give you error messages.

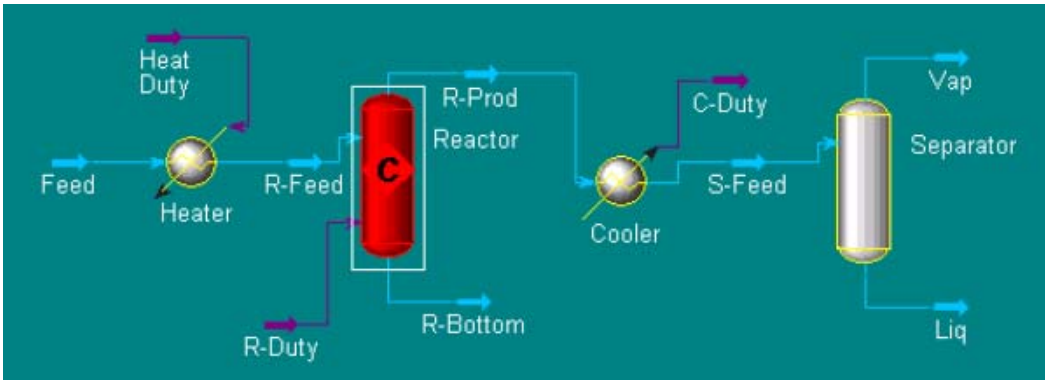


Figure 13-1

13.2 Example 2: Modification of Process for the Improvement

Inspection of the calculation results of Example 1 shows that the cooling duty is comparable to the heating duty, suggesting that the utility load can be reduced by preheating the feed stream with hot reactor product. Modify the process by adding a heat exchanger. This can be accomplished in the *PFD* using the following steps:

1. Click Heater of *PFD* and change the name of the feed stream to Pre-Heat. Close the window.
2. Click the R-Prod stream of *PFD*. *Worksheet* of the outlet stream will pop up. Change the name of the Reactor effluent stream to R-Prod1.
3. Click Cooler of *PFD* and change the name of the feed stream to R-Prod2.
4. Install the Pre-Heater unit, using the Heat-exchanger model, with Feed and Pre-Heat as the tube-side inlet and outlet streams, and with R-Prod1 and R-Prod2 as the shell-side inlet and outlet streams. Click **Parameter** at the left side of the window. Specify Delta p as 0 for both tube side and shell side. Choose Weighted Exchanger as Model. Close the window.
5. You still need to specify one more condition. Open the *Worksheet* and specify the temperature of Pre-Heat stream to 600 F. You may change this temperature to see how it affects the Heat-duty.
6. You can change the Pre-Heat stream temperature and see how it affects the H-Duty and UA (heat transfer coefficient x interfacial area). Increasing Pre-Heat temperature can reduce the H-Duty, but it will increase UA, which means that you need a heat exchanger with more interfacial area (bigger and with more inner pipes). Obviously, there will be upper limit of Pre-Heat temperature no matter how good your heat exchanger is. You can see this effect by changing the temperature and recording the change of other values. This can be done by using *Databook* function (under the *Tools* pull down menu.). The process can be described as follows:
   a. Open *Tools/Databook*. Click **Insert** button and choose **Pre-Heat** as object, **Temperature** as Variable and click **Add** button. Do the same for **Heat-Duty** as object, **Heat Flow** as Variable and **Heat Exch** as object, **UA** as Variable. Close the window.
   b. Go to the **Case Studies** page and click **Add.** Check **Ind** (Independent variable) for **Pre-Heat** and check **Dep** (Dependant variable) for **Heat-Duty** and **Heat Exch.** Click **View.** Type in **500** for Low Bound, **620** for High Bound, and **10** for Step Size.
   c. Click **Start**. After a few seconds, click **Results.**

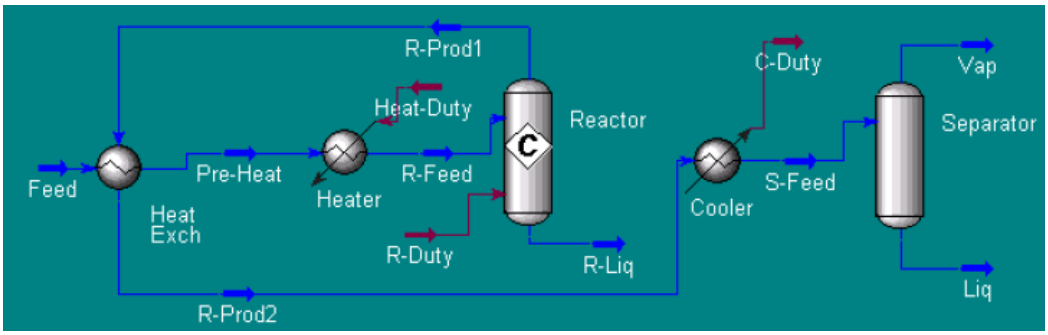


Figure 13-2

13.3 Example 3: Process Involving Recycle

Ethyl chloride will be produced by the gas-phase reaction of HCl with ethylene over a copper chloride catalyst supported on silica as

$$C_2H_4 + HCl \rightarrow C_2H_5Cl$$

The feed stream is composed of 50 mol% HCl, 48 mol% C_2H_4, and 2 mol% N_2 at 100 kmol/hr, 25 ^oC, and 1 atm. Since the reaction achieves only 90 mol% conversion, the ethyl chloride product is separated from the unreacted reagents, and the latter is recycled. The separation is achieved using a distillation column, where it is assumed that a perfect separation is achievable. The process is operated at atmospheric pressure, and pressure drops are ignored. To prevent the accumulation of inerts in the system, 10 kmol/hr is withdrawn in a purge stream, W. Show the effect of the flowrate of the purge stream W on the recycle R and on the composition of the reactor feed.

Solution

This instruction is brief. You may not be able to understand it unless you have finished the previous chapters.

1. Start HYSYS and choose **Peng Robinson** as Base Property Package. Open **Component** page of *Fluid Package* window and add components (ethylene (or ethene), hydrogen_chloride, ethyl_chloride, and nitrogen) and close the *Fluid Package.*
2. Click **Enter Simulation Environment** and click **Mixer** in the *Object Palette* and click it on *Process Flow Diagram (PFD)*. Do the same for the **Conversion Reactor**, **Component Splitter, Tee** (Tee is at the right side of mixer in *Object Pallette*), and **Recycler** as shown in the Figure 13.3.
3. Name all streams as shown in the Figure 13.3.
4. Click Flowsheet/Reaction Package. Add Global Rxn Set. Then, click Add Rxn at the lower right side of the window and choose Conversion. Add three components (ethylene, hydrogen_chloride, and ethyl_chloride) and Stoich Coeff (-1, -1, 1). Click Basis page, and type 90 for Co for Ethylene as a basis. Close windows until you see PFD.
5. Double click the Conversion Reactor. Choose Global Rxn Set as Reaction set and close the window.
6. Double click the Recycle and set your Parameter/Tolerance to be all "1."
7. Since it was assumed that the components were separated perfectly, ethyl chloride was recovered in the bottom at 100% purity, with the other three components in the overhead product. This can be specified by double clicking Component Splitter and Clicking Splits (Under Design) and filling in 0 for ClC_2 and 1's for other three components.
8. Now open *Workbook*. Check the units to see if it is in SI units. Otherwise, change the unit by clicking Tools/Preferences/Variables. Choose **SI** and click **Clone** and change the units so that it is most convenient to you.
9. Fill in the *Workbook* with all the given condition, starting from the Feed stream: temperature (25 ^oC), pressure (1 atm), and molar flow (100 kmol/hr). Double click 100 (molar flow rate), and fill in the composition and close.
10. Continue to fill in the Workbook for the R* stream with the flow rate of zero and the condition and composition equal to those of the feed, to allow computations to proceed. Fill in the temperature (25 ^oC) of the streams S3, S4, and P. Fill in the pressure (1 atm) of the streams S4 and P.

11. Specify the molar flow rate of the stream of W to be 10 kmol/hr. Now you can open the Worksheet to see the result of the calculation.

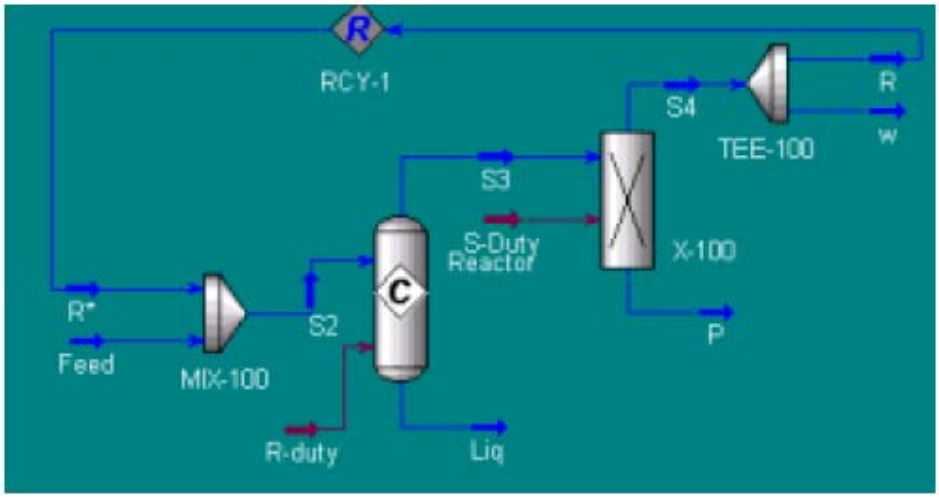


Figure 13-3

13.4 Example 4: Ethylene Oxide Process

The ethylene oxide process considered in this study can be described as follows:
A fresh feed stream consisting of ethylene gas (63 mol %) and pure O_2 gas (37 mol %) at 20 ^oC and 303 kPa enters an oxidation reactor system with a molar flowrate of 120 kmol/hr plus recycled gasses/vapors (estimated by HYSYS). The reaction is promoted by a solid catalyst and occurs **isothermally** at 230 ^oC. The feed stream must therefore be **pre-heated** to 230 ^oC before it is fed into the oxidation reactor.

The reaction is fairly selective, but is accompanied by a side-reaction that burns ethylene into catalytic combustion products. The combined stoichiometry is thus:

Selective reaction $C_2H_4 + 0.5O_2 \rightarrow C_2H_4O$

Side reaction $C_2H_4 + 3O_2 \rightarrow 2CO_2 + 2H_2O$

In the selective reaction, oxygen is the key reactant (basis for conversion) and its conversion is 80%, whereas in the side reaction, the conversion of oxygen is 19%. The pressure drop across the reactor is 70 kPa.

The hot effluent is cooled to -1^oC (in practice this very large temperature difference can only achieved by direct contact heat exchange, ie a quench system). The pressure drop across the large condenser is 50 kPa. Under these conditions, the product stream has a vapour fraction of about 0.8 and the task of recovering condensable liquid ethylene oxide begins. The cool product stream is fed into a **3-phase separator** and the light liquid phase is separated from the heavy liquid phase and vapour residual. HYSYS normally puts water in the heavy phase when there is a non-zero water stream.

The vapour residual is rich in ethylene but also contains recoverable ethylene oxide. Thus this vapour residual is further cooled to -30 ^oC to decrease its vapour fraction (pressure drop across cooler 10 kPa) and the cooled stream fed into a 2 phase separator (flash drum). The liquid stream rich in ethylene oxide is mixed with the organic-aqueous stream from the 3-phase separator (the combined stream pressure is set to the lowest of the feeds) and the combined stream fed into a conventional distillation column. The column has a partial condenser and its duty would be to obtain almost pure ethylene oxide liquid product (>99% mol). The vapor stream leaving the flash drum is throttled down to 101 kPa with a throttling valve before being fed into a component splitter (a packed column with a special alumina packing to adsorb CO_2/O_2 from the stream and leave ethylene and any residual ethylene oxide). In practice this operation is a pressure swing column where CO_2/O_2 are flushed out by high temperature low pressure desorption). The organic gas/vapor stream rich in ethylene is first compressed to 303 kPa and recycled back to the feed to the reactor (it is mixed with fresh feed of ethylene/O_2). In the HYSYS model a recycle logic operation is required. This computational unit will calculate the recycle flowrate. Usually when the recycle unit is installed, the initial recycle flow is set to zero because it is not known.

Use HYSYS to produce a flowsheet for the process described. For this task, use the following information alongside details provided earlier:

(a) Employ the **NRTL** activity model for liquids and **SRK** for the vapor phase.
(b) Employ a "conversion reactor" in the HYSYS model (guidance available on the handout)
(c) The **column** will have a partial condenser and 12 stages with a feed located at stage 6.
(d) The **column** condenser pressure will be 101 kPa and the reboiler pressure will be 160 kPa

(e) For **column** solution (you will be doing rigorous stage to stage calculations), employ the following **initial specifications**:
   1- Full recovery of water at the bottom of the column (mole fraction of 1 specified)
   2- 90% recovery of ethylene oxide (0.9 mol frac) in the overhead liquid (OUR FINAL PRODUCT)
   3- 90% recovery of ethylene gas (0.90 mol frac) in the overhead vapour. Make sure the degree of freedom is zero.

(f) For the **component splitter**, use the following info: Overhead pressure and vapor fraction 101 kPa and 1 respectively; and bottoms pressure and vapor fraction 101 kPa and 1 respectively.

(g) For the recycle operation, use **zero as an initial guess** for the recycle flowrate. HYSYS will find the correct value by iterations.