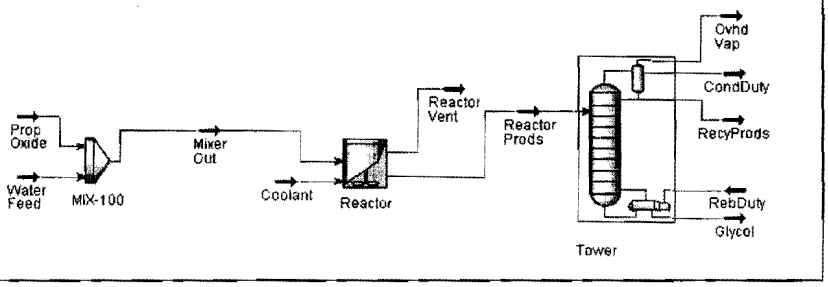
3 Chemicals Tutorial

3.1 Introduction

The complete case for this tutorial has been pre-built and is located in the file **TUTOR3.HSC** in your **HYSYS\Samples** directory.

In this tutorial, 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 reactor outlet stream is then fed to a distillation tower, where essentially all the glycol is recovered in the tower bottoms. A flowsheet for this process appears below.

Figure 3.1



The following pages will guide you through building a HYSYS case for modeling this process. This example will illustrate the complete construction of the simulation, including selecting a property package and components, defining the reaction, installing streams and unit operations, and examining the final results. The tools available in HYSYS interface will be utilized to illustrate the flexibility available to you.

Before proceeding, you should have read Chapter A - HYSYS Tutorials which precedes the tutorials in this manual.

3.2 Steady State Simulation

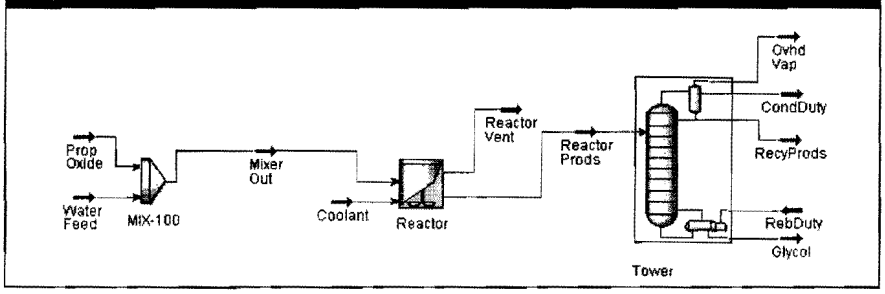
3.2.1 Process Description

The simulation will be built using these basic steps:

1. Create a unit set.
2. Choose a property package.
3. Select the components.
4. Define the reaction.
5. Create and specify the feed streams.
6. Install and define the Mixer and Reactor.
7. Install and define the Distillation Column.

The process being modeled in this example is the conversion of propylene oxide and water to propylene glycol in a CSTR Reactor. The reaction products are then separated in a distillation tower. A flowsheet for this process appears below.

Figure 3.2



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. The Reactor product stream is fed to a distillation tower, where essentially all the glycol is recovered in the bottoms product.

The Workbook displays information about streams and unit operations in a tabular format, while the PFD is a graphical representation of the flowsheet.

The two primary building tools, Workbook and PFD, are used to install the streams and operations, and to examine the results while progressing through the simulation. Both of these tools provide you with a large amount of flexibility in building your simulation and in quickly accessing the information you need.

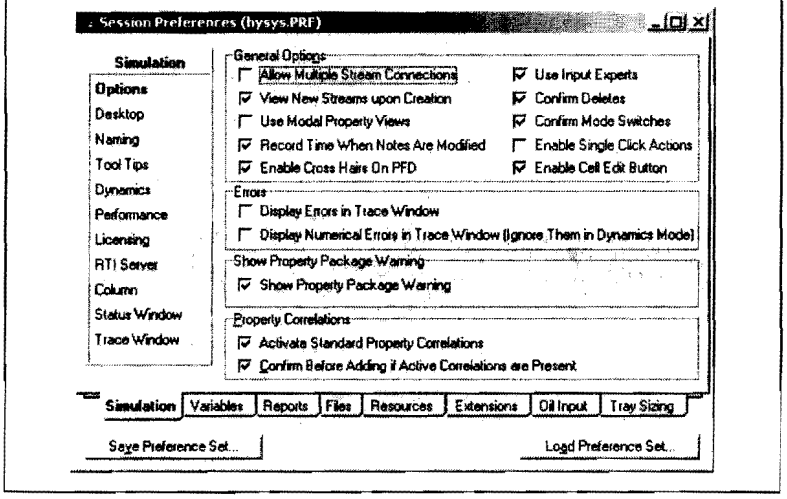
The Workbook is used to build the first part of the flowsheet, including the feed streams and the mixer. The PFD is then used to install the reactor, and a special sequence of views called the Input Expert will be used to install the distillation column.

3.2.2 Setting Your 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 view appears.

Figure 3.3



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.

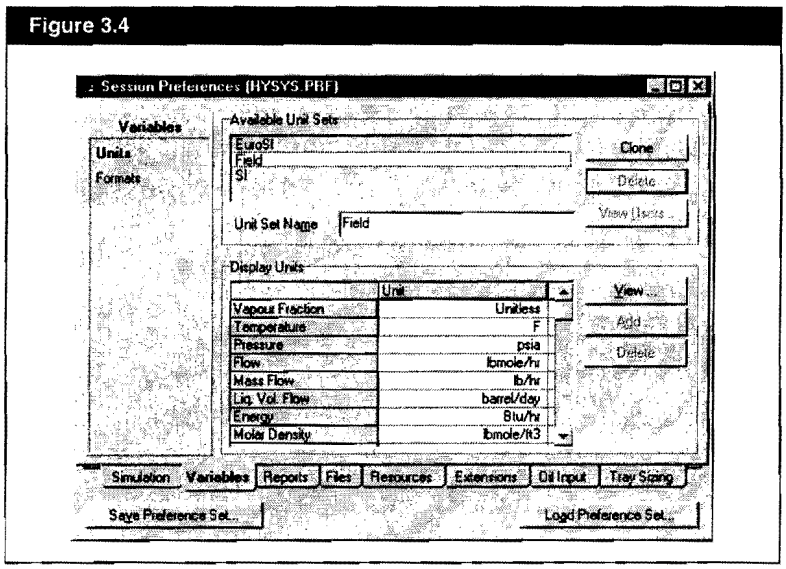
Creating a New Unit Set

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 tutorial, you will create a new unit set based on the HYSYS Field set, then customize it

1. In the Available Units Sets 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 3.4

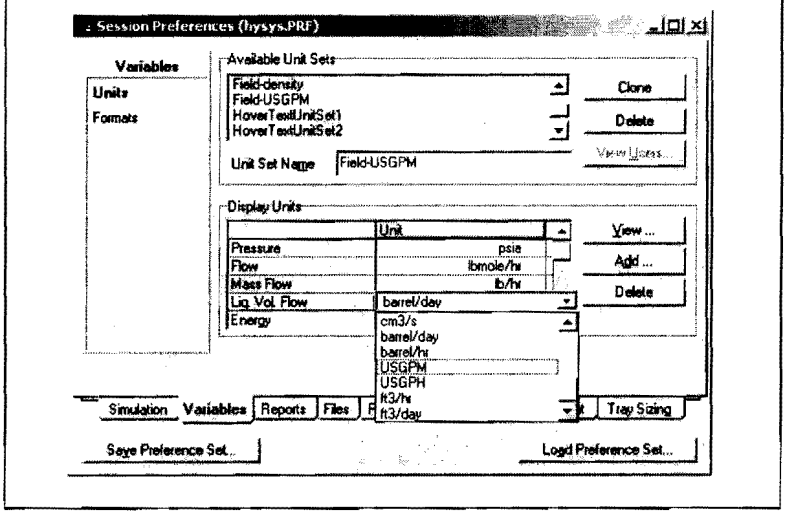


The default Preference file is named **HYSYS.prf**. When you modify any of the preferences, you can save the changes in a new Preference file by clicking the **Save Preference Set** button. HYSYS prompts you to provide a name for the new Preference file, which you can later recall into any simulation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

2. Click the **Clone** button. A new unit set named NewUser appears in the Available Unit Sets list.
3. In the **Unit Set Name** field, 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 3.5



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

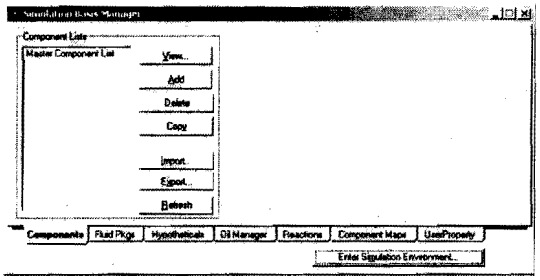
3.2.3 Defining the Fluid Package

New Case Icon

1. Click the **New Case** icon.
2. The Simulation Basis Manager appears.

All commands accessed via the tool bar are also available as menu items.

Figure 3.6



HYSYS displays the current **Environment** and **Mode** in the upper right corner of the view. Whenever you begin a new case, you are automatically placed in the **Basis** Environment, where you can define your property package and components.

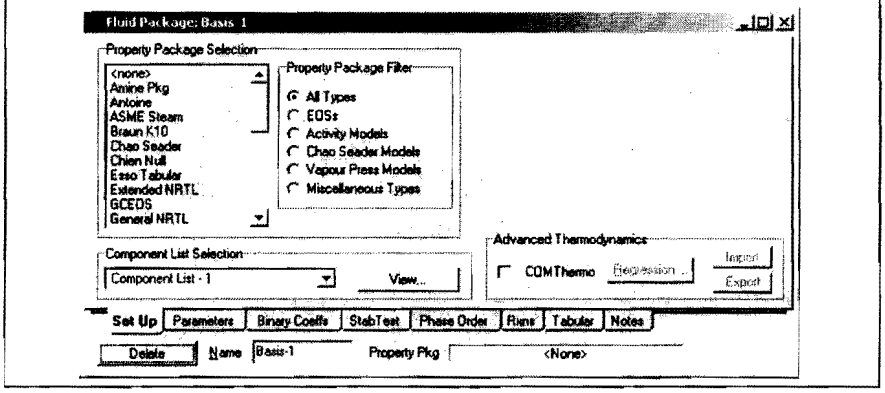
The next task is to create a Fluid Package. A Fluid Package, at minimum, contains the components and property method that HYSYS will use in its calculations for a particular flowsheet. Depending on what a specific flowsheet requires, a Fluid Package may also contain other information such as reactions and interaction parameters.

Creating a Fluid Package

1. Click the **Fluid Pkgs** tab of the Simulation Basis Manager.
2. Click the **Add** button. The Fluid Package property view appears.

The Simulation Basis Manager allows you to create, modify, and otherwise manipulate Fluid Packages in your simulation case. Most of the time, as with this example, you will require only one Fluid Package for your entire simulation.

Figure 3.7



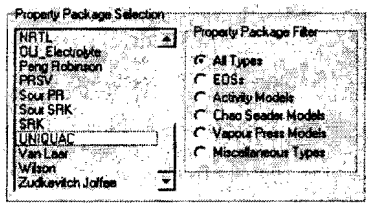
HYSYS has created a Fluid Package with the default name **Basis-1**. You can change the name of this fluid package by typing a new name in the **Name** cell at the bottom of the view.

The Fluid Package property view allows you to supply all the information required to completely define the Fluid Package. In this tutorial you will use the following tabs: Set Up, Binary Coeffs (Binary Coefficients), and Rxns (Reactions).

You choose the Property Package on the Set Up tab. The currently selected property package is <none>. There are a number of ways to select the desired base property package, in this case UNIQUAC.

3. Do **one** of the following:
   - Begin typing UNIQUAC, and HYSYS finds the match to your input.
   - Use the vertical scroll bar to move down the list until UNIQUAC becomes visible, then click on it.

Figure 3.8

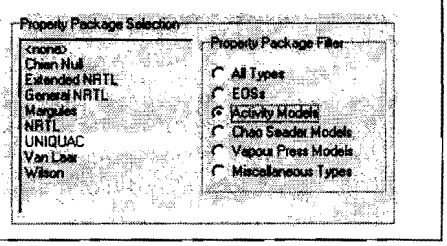


The Property Pkg indicator bar at the bottom of the view now indicates UNIQUAC is the current property package for this Fluid Package.

Figure 3.9

Alternatively, you can select the Activity Models radio button in the Property Pkg Filter group, producing a list of only those property packages which are Activity Models. UNIQUAC appears in the filtered list, as shown here.

Figure 3.10



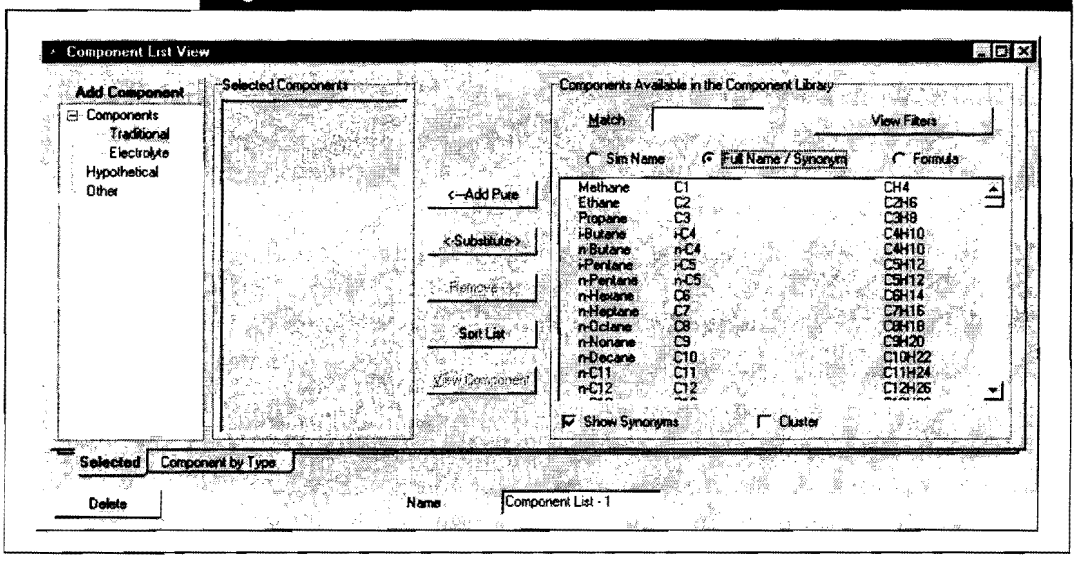
In the Component List Selection drop-down list, HYSYS filters to the library components to include only those appropriate for the selected Property Package. In this case, no components have yet been defined.

Selecting Components

Now that you have chosen the property package to be used in the simulation, your next task is to select the components.

1. In the Component List Selection group, click the **View** button. The Component List View appears.

Figure 3.11



Each component can appear in three forms, corresponding to the three radio buttons that appear above the component list.

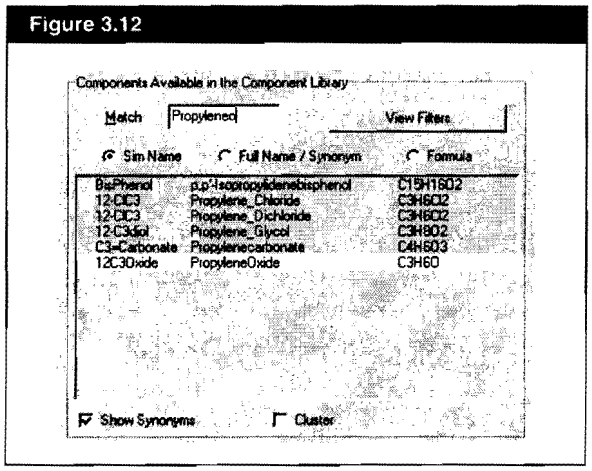
Feature	Description
SimName	The name appearing within the simulation.
FullName/Synonym	IUPAC name (or similar), and synonyms for many components.
Formula	The chemical formula of the component. This is useful when you are unsure of the library name of a component, but know its formula.

Based on the selected radio button, HYSYS locates the component(s) that best matches the information you type in the Match field.

In this tutorial you will use propylene oxide, propylene glycol and H2O. First, you will add propylene oxide to the component list.

2. Ensure the **SimName** radio button is selected and the **Show Synonyms** checkbox is checked.
3. In the **Match** field, start typing propyleneoxide, as one word. HYSYS filters the list as you type, displaying only those components that match your input.

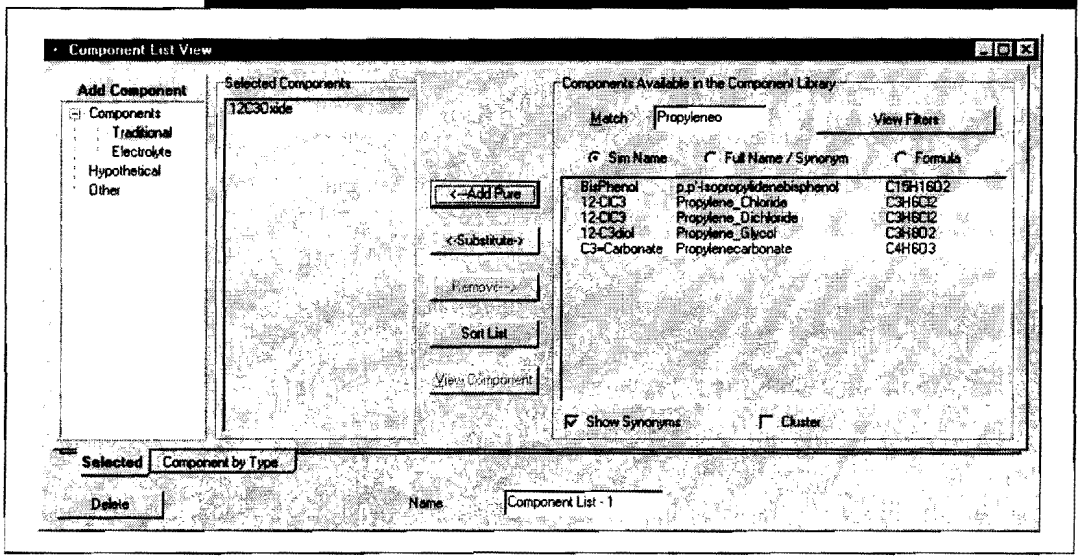
Figure 3.12

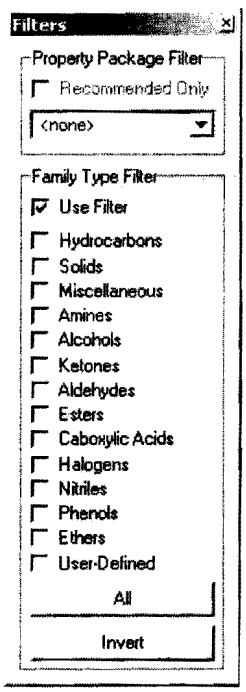


4. When propylene oxide is selected in the list, add it to the Selected Components List by doing one of the following:
   - Press the **ENTER** key.
   - Click the **Add Pure** button.
   - Double-click on **PropyleneOxide**.

The component now appears in the Selected Components List.

Figure 3.13





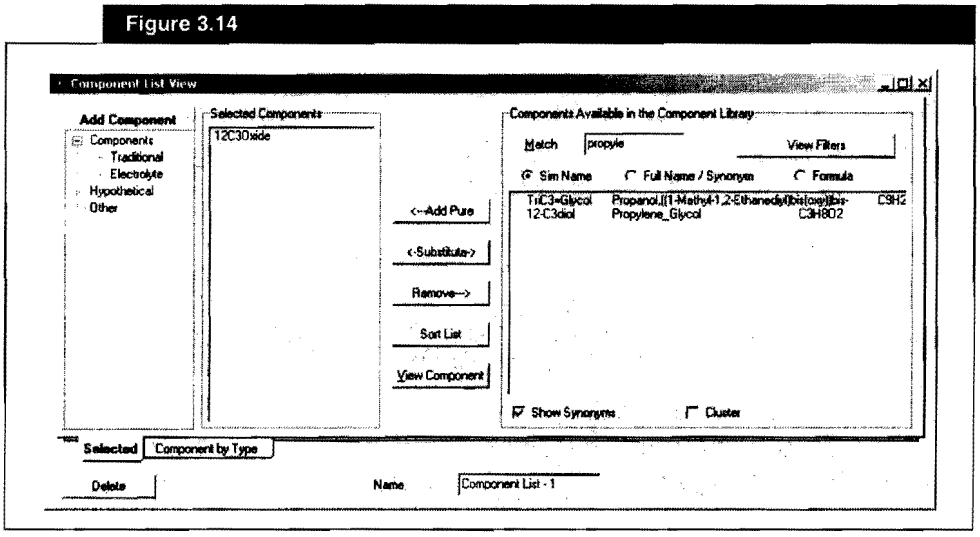
Another method for finding components is to use the View Filters to display only those components belonging to certain families.

Next, you will add Propylene Glycol to the component list using the filter.

5. Ensure the **Match** field is empty by pressing ALT M and then the DELETE key.
6. Click the **View Filters** button. The Filters view appears.
7. Click the **Use Filter** checkbox to activate the filter checkboxes.
8. Since Propylene Glycol is an alcohol, click the **Alcohols** checkbox.

9. In the **Match** field, begin typing propyleneglycol, as one word. HYSYS filters as you type, displaying only the alcohols that match your input.

Figure 3.14



10. When Propylene Glycol is selected in the list, press the ENTER key to add it to the Selected Components list.

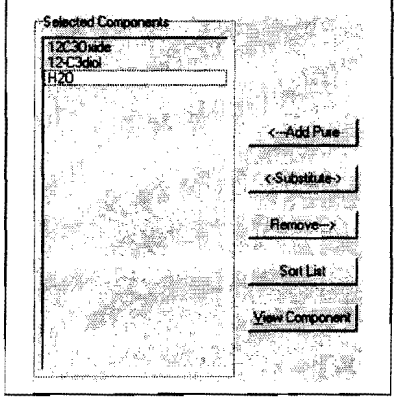
Finally, you will add the component H2O.

11. In the Filter view, clear the **Alcohols** checkbox by clicking on it.
12. Ensure the **Match** field is empty by pressing ALT M and then the DELETE key
13. H2O does not fit into any of the standard families, so click on the **Miscellaneous** checkbox.
14. Scroll down the filtered list until H2O is visible, then double-click on H2O to add it to the Selected Components list.

15. The final component list appears below.

A component can be removed from the Selected Components list by selecting it and clicking the **Remove** button or the **DELETE** key.

Figure 3.15

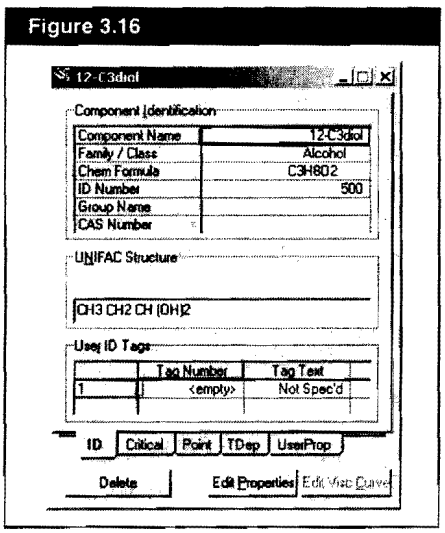


Viewing Component Properties

To view the properties of one or more components, select the component(s) and click the View Component button. HYSYS opens the property view(s) for the component(s) you select.

1. Click on 12C3diol in the Selected Components List.
2. Click the **View Component** button. The property view for the component appears.

Figure 3.16



The Component property view provides you with complete access to the pure component information for viewing only. You cannot modify any parameters for a library component, however, HYSYS allows you to clone a library component into a Hypothetical component, which can then be modified as desired. Refer to **Chapter 3 - Hypotheticals** in the Simulation Basis manual for more information on cloning library components.

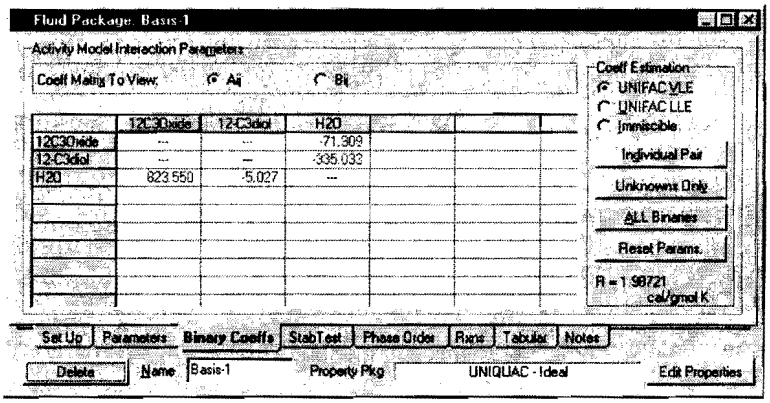
3. Close the individual component view, then close the Component List View to return to the Fluid Package.

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 view..

Figure 3.17



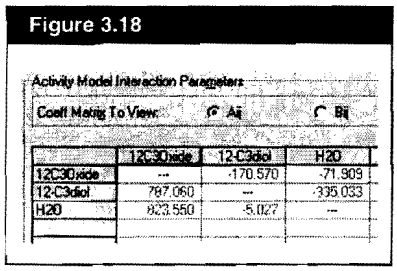
In the Activity Model Interaction Parameters group, the Aij interaction table appears by default. HYSYS automatically inserts the coefficients for any component pairs for which library data is available. You can change any of the values provided by HYSYS if you have data of your own.

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, for this example, you will use one of HYSYS' built-in estimation methods instead.

Next, you will use the UNIFAC VLE estimation method to estimate the unknown pair.

2. In the Coeff Estimation group, ensure the **UNIFAC VLE** radio button is selected.
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 3.18



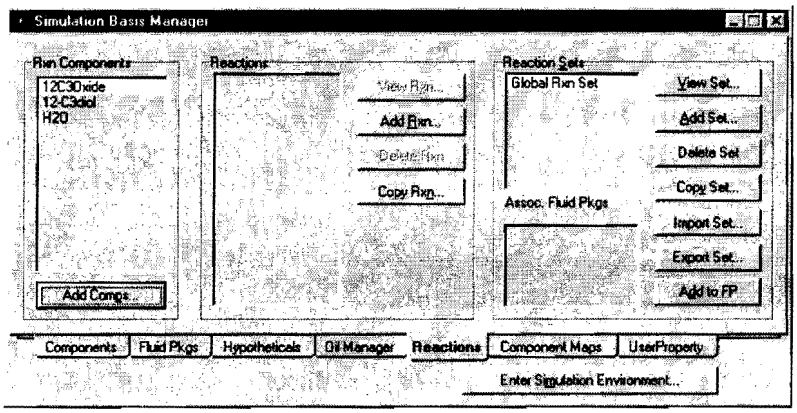
4. To view the Bij coefficient table, select the **Bij** radio button. For this example, all the Bij coefficients will be left at the default value of zero.

3.2.4 Defining the Reaction

Basis Icon

1. Return to the Simulation Basis Manager view by clicking on its title bar, or by clicking the **Basis** icon.
2. Click the **Reactions** tab. This tab allows you to define all the reactions for the flowsheet.

Figure 3.19



The reaction between water and propylene oxide to produce propylene glycol is as follows:

$$H_2O + C_3H_6O \rightarrow C_3H_8O_2 \qquad (3.1)$$

These steps will be followed in defining our reaction:

1. Create and define a Kinetic Reaction.
2. Create a Reaction Set containing the reaction.
3. Activate the Reaction set to make it available for use in the flowsheet.

Selecting the Reaction Components

The first task in defining the reaction is choosing the components that will be participating in the reaction. In this tutorial, all the components that were selected in the Fluid Package are participating in the reaction, so you do not have to modify this list. For a more complicated system, however, you would add or remove components from the list.

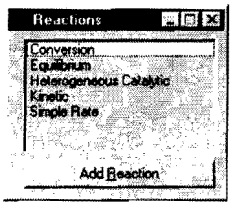
To add or remove a component, click the Add Comps button. The Component List View appears. Refer to the **Selecting Components** section in **Section 3.2.3 - Defining the Fluid Package** for more information.

Creating the Reaction

Once the reaction components have been chosen, the next task is to create the reaction.

1. In the Reactions group, click the **Add Rxn** button. The Reactions view appears.

Figure 3.20

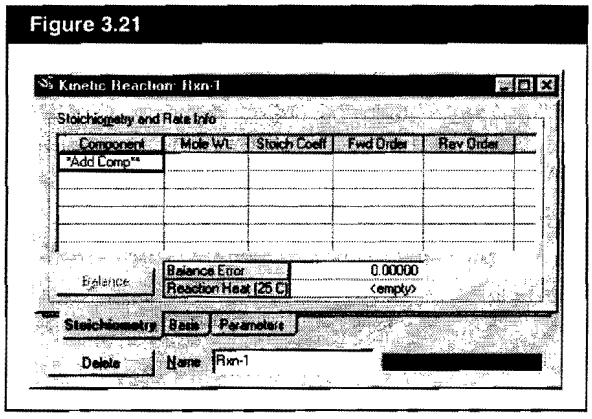


2. In the list, select the Kinetic reaction type, then click the **Add Reaction** button. The Kinetic Reaction property view appears, opened to the **Stoichiometry** tab.

On the Stoichiometry tab, you can specify which of the Rxn Components are involved in the particular reaction as well as the stoichiometry and the reaction order.

Often you will have more than one reaction occurring in your simulation case. On the Stoichiometry tab of each reaction, select only the Rxn Components participating in that reaction.

Figure 3.21

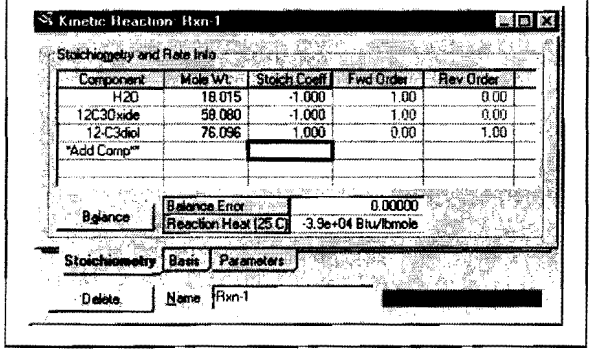


3. In the Component column, click in the cell labeled ****Add Comp****.
4. Select Water as a reaction component by doing **one** of the following:
   - Open the drop-down list and select H2O from the list of available reaction components.
   - Type H2O. HYSYS filters as you type, searching for the component which matches your input. When H2O is selected, press the **ENTER** key to add it to the Component list.
5. Repeat this procedure to add 12C3Oxide and 12-C3diol to the reaction table.

The next task is to enter the stoichiometric information. A negative stoichiometric coefficient indicates that the component is consumed in the reaction, while a positive coefficient indicates the component is produced.

6. In the Stoich Coeff column, click in the **<<empty>>** cell corresponding to H2O.
7. Type -1 and press the ENTER key.
8. Enter the coefficients for the remaining components as shown in the view below:

Figure 3.22



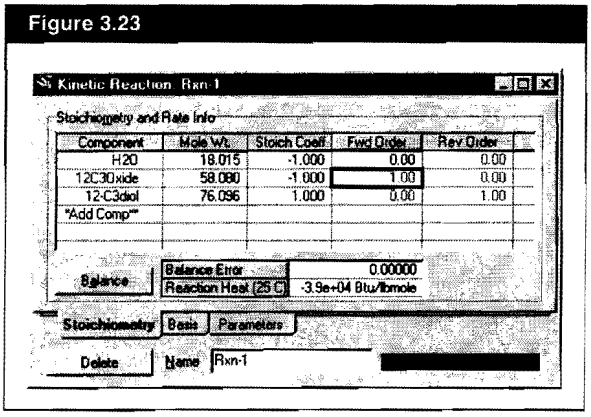
Once the stoichiometric coefficients are supplied, the Balance Error cell will show 0 (zero), indicating that the reaction is mass balanced. HYSYS will also calculate and display the heat of reaction in the Reaction Heat cell. In this case, the Reaction Heat is negative, indicating that the reaction produces heat (exothermic).

HYSYS provides default values for the Forward Order and Reverse Order based on the reaction stoichiometry. The kinetic data for this Tutorial is based on an excess of water, so the kinetics are first order in Propylene Oxide only.

9. 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.

Notice that the default values for the Forward Order and Reverse Order appear in red, indicating that they are suggested by HYSYS. When you enter the new value for H2O, it will be blue, indicating that you have specified it.

Figure 3.23



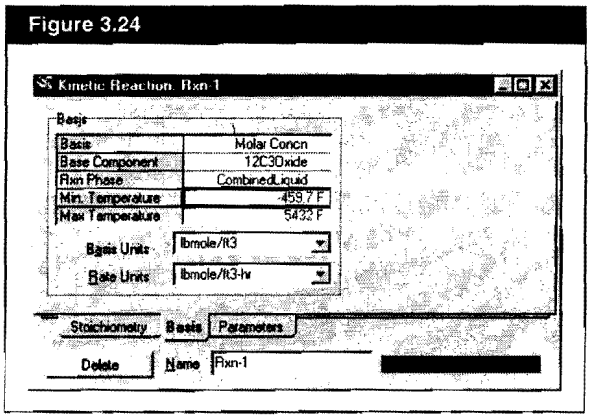
The next task is to define the reaction basis.

10. In the Kinetic Reaction view, click the **Basis** tab.
11. In the **Basis** cell, accept the default value of Molar Concn.
12. Click in the **Base Component** cell. By default, HYSYS has chosen the first component listed on the **Stoichiometry** tab, in this case H2O, as the base component.
13. Change the base component to Propylene Oxide by doing **one** of the following:
    - Open the drop-down list of components and select 12C3Oxide.
    - Begin typing 12C3Oxide, and HYSYS filters as you type. When 12C3Oxide is selected, press the **ENTER** key.

You can have the same reaction occurring in different phases with different kinetics and have both calculated in the same **REACTOR**.

14. In the **Rxn Phase** cell, select CombinedLiquid from the drop-down list. The completed **Basis** tab appears below.

Figure 3.24

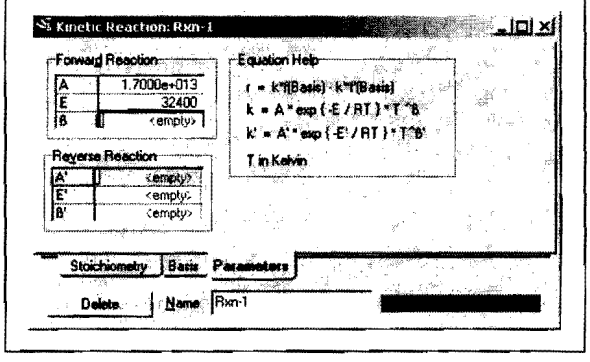


The Min. Temperature, Max. Temperature, Basis Units and Rate Units are acceptable at their default values.

15. 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:
16. In the Forward Reaction **A** cell, enter 1.7e13.
17. 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.

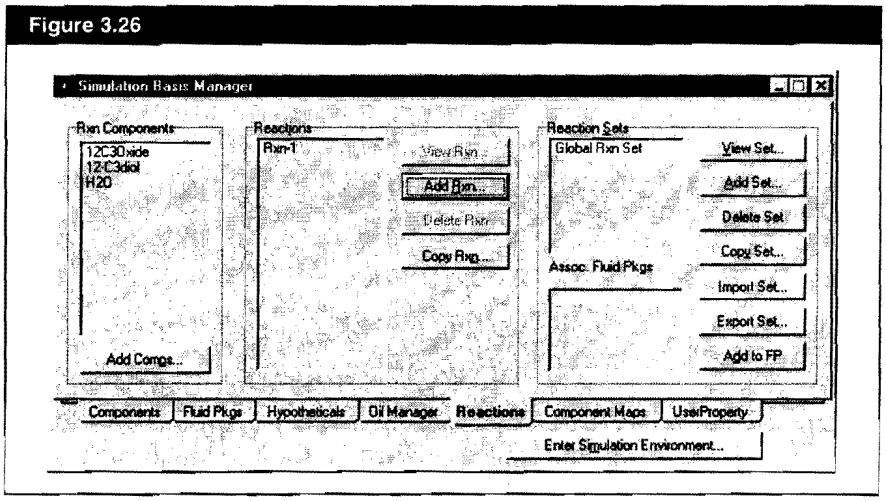
Figure 3.25



18. Close both the Kinetic Reaction property view and the Reactions view.
19. Click the **Basis** icon to ensure the Simulation Basis Manager view is active. On the **Reactions** tab, the new reaction, Rxn-1, now appears in the Reactions group.

Basis Icon

Figure 3.26



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 (Global Reaction Set) which contains all of the reactions you have defined. In this tutorial, since there is only one REACTOR, the default Global Rxn Set could be attached to it, however, for illustration purposes, a new reaction set will be created.

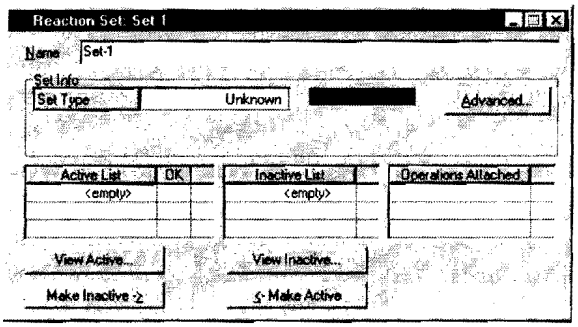
Creating a Reaction Set

The same reaction(s) can be in multiple Reaction Sets.

Reaction Sets provide a convenient way of grouping related reactions. For example, consider a flowsheet in which a total of five reactions are taking place. In one REACTOR operation, only three of the reactions are occurring (one main reaction and two side reactions). You can group the three reactions into a Reaction Set, then attach the set to the appropriate REACTOR unit operation.

1. In the Reaction Sets group, click the **Add Set** button. The Reaction Set property view appears with the default name Set-1.

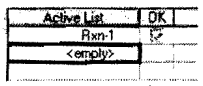
Figure 3.27



The drop-down list contains all reactions in the Global Reaction Set. Currently, **Rxn-1** is the only reaction defined, so it is the only available selection.

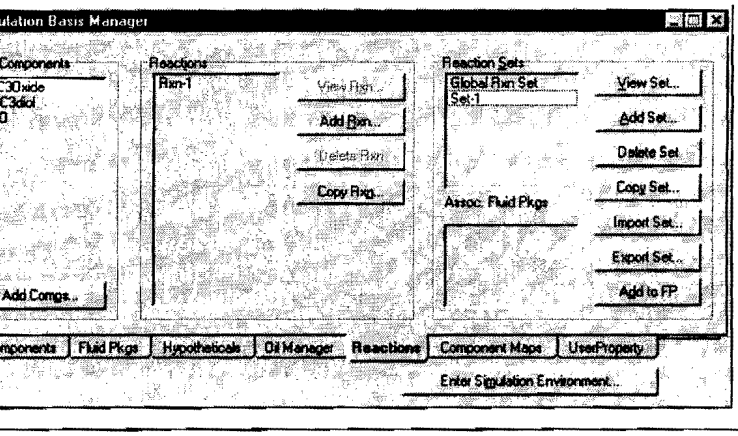
2. In the Active List, click in the cell labeled **<empty>**.
3. Open the drop-down list and select Rxn-1.

A checkbox labeled OK automatically appears next to the reaction in the Active List. The reaction set status bar changes from Not Ready to Ready, indicating that the new reaction set is complete.



4. Close the Reaction Set view to return to the Simulation Basis Manager. The new reaction set named Set-1 now appears in the Reaction Sets group.

Figure 3.28

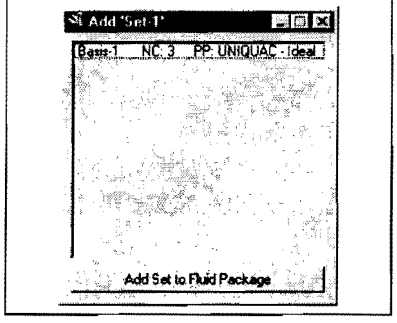


Making the Reaction Set Available to the Fluid Package

The final task is to make the set available to the Fluid Package, which also makes it available in the flowsheet.

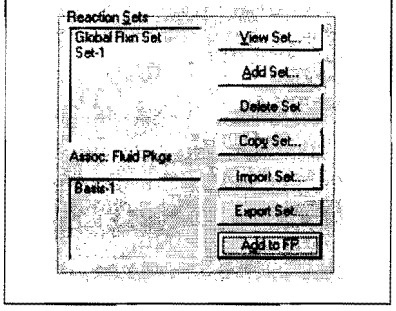
1. Click on **Set-1** in the Reaction Sets group on the Reactions tab.
2. Click the **Add to FP** button. The Add 'Set-1' view appears. This view prompts you to select the Fluid Package to which you would like to add the reaction set. In this example, there is only one Fluid Package, Basis-1.

Figure 3.29



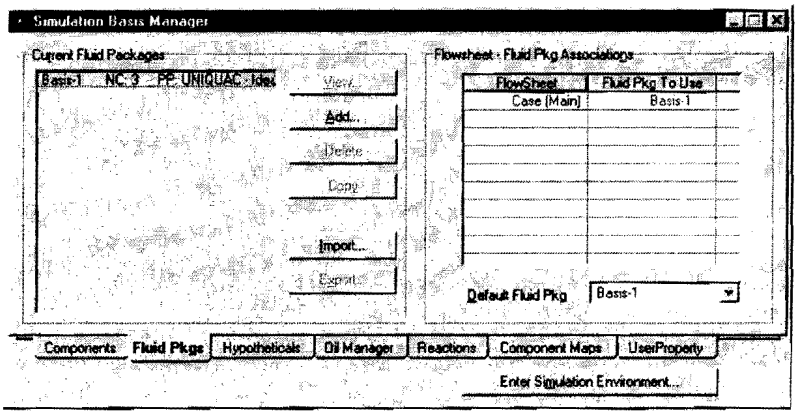
3. Select Basis-1, then click the **Add Set to Fluid Package** button.

Figure 3.30



4. Click the **Fluid Pkgs** tab to view a summary of the completed Fluid Package.

Figure 3.31



The list of Current Fluid Packages displays the new Fluid Package, Basis-1, showing the number of components (NC) and property package (PP). The new Fluid Package is assigned by default to the Main Simulation, as shown in the Flowsheet-Fluid Pkg Associations group. Now that the Basis is defined, you can install streams and operations in the Simulation environment (also referred to as the Parent Simulation environment or Main Simulation environment).

3.2.5 Entering the Simulation Environment

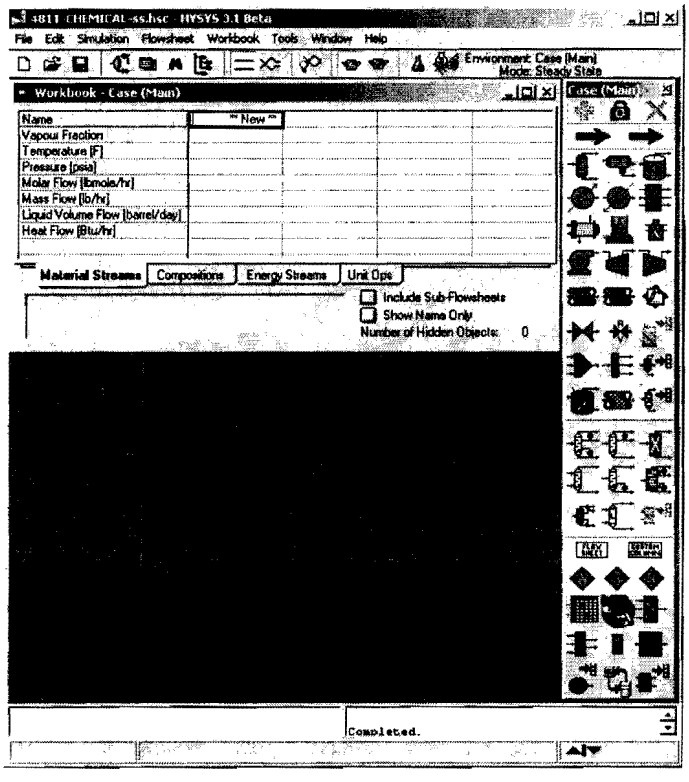
Enter Simulation Environment Icon

To leave the Basis environment and enter the Simulation environment, do one of the following:

- Click the **Enter Simulation Environment** button on the Simulation Basis Manager.
- Click the **Enter Simulation Environment** icon on the toolbar.

When you enter the Simulation environment, the initial view that appears is dependent on your current preference setting for the Initial Build Home View. Three initial views are available, namely the PFD, Workbook and Summary. Any or all of these can be displayed at any time, however, when you first enter the Simulation environment, only one is displayed. For this example, the initial Home View is the Workbook (HYSYS default setting).

Figure 3.32



There are several things to note about the Main Simulation environment. In the upper right corner, the Environment has changed from Basis to Case (Main). A number of new items are now available on the Menu and Toolbar, and the Workbook and Object Palette are open on the Desktop. These two latter objects are described below.

Features	Description
Workbook	A multiple-tab view containing information about the objects (streams and unit operations) in the simulation case. By default, the Workbook has four tabs, namely Material Streams, Compositions, Energy Streams and Unit Ops. You can edit the Workbook by adding or deleting tabs and changing the information displayed on any tab.
Object Palette	A floating palette of buttons that can be used to add streams and unit operations.

You can toggle the palette open or closed by pressing **F4**, or by choosing **Open/Close Object Palette** from the Flowsheet menu.

Before proceeding any further to install streams or unit operations, save your case.

1. Do one of the following:
   - Click the **Save** icon on the toolbar.
   - From the **File** menu, select **Save**.
   - Press **CTRL S**.

Save Icon

If this is the first time you have saved your case, the Save Simulation Case As view appears. By default, the File Path is the Cases sub-directory in your HYSYS directory.

Open Case Icon

When you choose to open an existing case by clicking the **Open Case** button, or by selecting **Open Case** from the **File** menu, HYSYS allows you to retrieve backup (*.**bk***) and HYSIM (*.**sim**) files in addition to standard HYSYS (*.**hsc**) files.

2. In the **File Name** cell type a name for the case, for example GLYCOL. You do not have to enter the.**hsc** extension; HYSYS automatically adds it for you.
3. Once you have entered a file name, press the **ENTER** key or the **OK** button. HYSYS will now save the case under the name you have given it when you Save in the future. The Save As view will not appear again unless you choose to give it a new name using the Save As command.

If you enter a name that already exists in the current directory, HYSYS will ask you for confirmation before over-writing the existing file.

3.2.6 Using the Workbook

Installing the Feed Streams

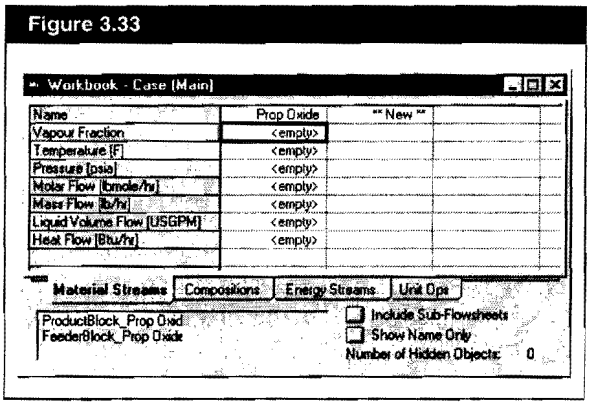
In general, the first task you perform when you enter the Simulation environment is to install one or more feed streams. In this section, you will install feed streams using the Workbook.

Workbook Icon

HYSYS accepts blank spaces within a stream or operation name.

1. Click the **Workbook** icon on the toolbar to make the Workbook active.
2. On the **Material Streams** tab, click in the ****New**** cell in the Name row.
3. Type the new stream name Prop Oxide, then press ENTER. HYSYS automatically creates the new stream.

Figure 3.33



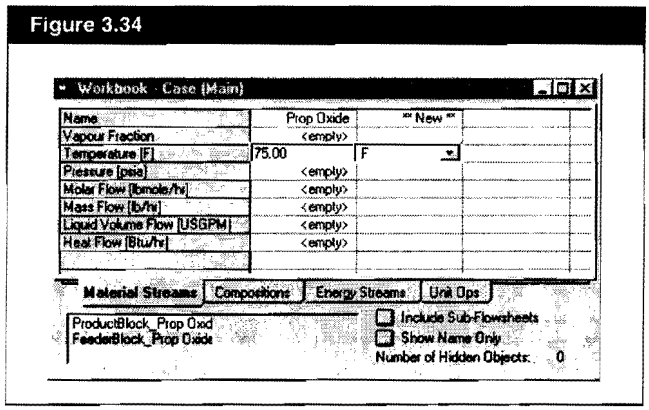
When you pressed ENTER after typing in the stream name, HYSYS automatically advanced the active cell down one cell, to Vapour Fraction.

Next you will define the feed conditions for temperature and pressure, in this case 75°F and 1.1 atm.

4. Click in the **Temperature** cell for Prop Oxide.

5. Type 75 in the **Temperature** cell. In the Unit drop-down list, HYSYS displays the default units for temperature, in this case F.

Figure 3.34

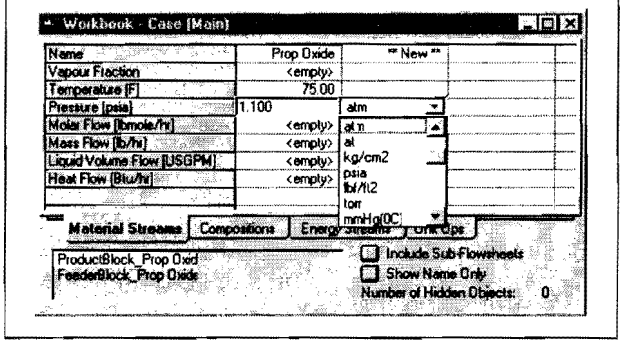


6. Since this is the correct unit, press ENTER.HYSYS accepts the temperature.
7. Click in the **Pressure** cell for Prop Oxide.

If you know the stream pressure in another unit besides the default of psia, HYSYS will accept your input in any one of a number of different units and automatically convert to the default for you. For example, you know the pressure of Prop Oxide is 1.1 atm.

8. Type 1.1.
9. Press the SPACEBAR or click on ▾. Begin typing 'atm'. HYSYS will match your input to locate the unit of your choice.

Figure 3.35



10. Once atm is selected in the list, press the ENTER key, and HYSYS accepts the pressure and automatically converts to the default unit, **psia**.

Alternatively, you can specify the unit simply by selecting it from the unit drop-down list.

11. Click in the **Molar Flow** cell for Prop Oxide, enter 150 lbmole/hr, then press ENTER.

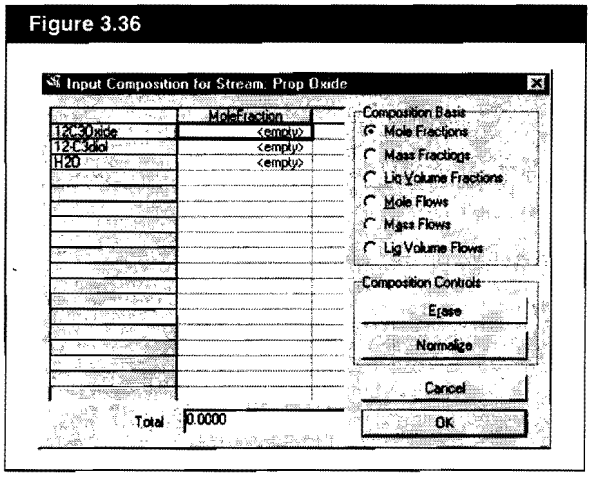
Providing Compositional Input

Now that the stream conditions have been specified, your next task is to input the composition.

12. In the Workbook, double-click the **Molar Flow** cell of the Prop Oxide stream.

    The Input Composition for Stream view appears. This view allows you to complete the compositional input.

Figure 3.36



The Input Composition for Stream view is Modal, indicated by the thick border and the absence of the **Minimize/Maximize** buttons in the upper right corner. When a Modal view is visible, you will not be able to move outside the view until you finish with it, by clicking either the **Cancel** or **OK** button.

The following table lists and explains the features available to you on the Input Composition for Stream view.

Features	Description
Compositional Basis Radio Buttons	You can input the stream composition in some fractional basis other than Mole Fraction, or by component flows, by selecting the appropriate radio button before providing your input.
Normalizing	The Normalizing feature is useful when you know the relative ratios of components; for example, 2 parts N2, 2 parts CO2, 120 parts C1, etc. Rather than manually converting these ratios to fractions summing to one, simply enter the individual numbers of parts and click the **Normalize** button. HYSYS computes the individual fractions to total 1.0. Normalizing is also useful when you have a stream consisting of only a few components. Instead of specifying zero fractions (or flows) for the other components, simply enter the fractions (or the actual flows) for the non-zero components, leaving the others <empty>. Click the **Normalize** button, and HYSYS forces the other component fractions to zero.
Calculation status/ colour	As you input the composition, the component fractions (or flows) initially appear in red, indicating the final composition is unknown. These values become blue when the stream composition is calculated. Three scenarios result in the stream composition being calculated: • Input the fractions of all components, including any zero components, such that their total is exactly 1.0000. Click the **OK** button. • Input the fractions (totalling 1.000), flows or relative number of parts of all non-zero components. Click the **Normalize** button, then click the **OK** button. • Input the flows or relative number of parts of all components, including any zero components, then click the **OK** button.

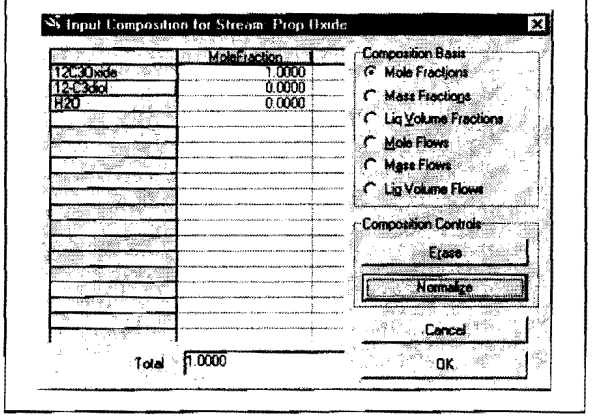
These are the default colours; yours may appear differently depending on your settings on the Colours page of the Session Preferences.

13. In the Composition Basis group, ensure that the **Mole Fractions** radio button is selected.
14. Click on the input cell for the first component, 12C3Oxide. This stream is 100% propylene oxide.
15. Type 1 for the mole fraction, then press ENTER.

In this case, 12C3Oxide is the only component in the stream.

16. Click the **Normalize** button to force the other values to zero. The composition is now defined for this stream.

Figure 3.37

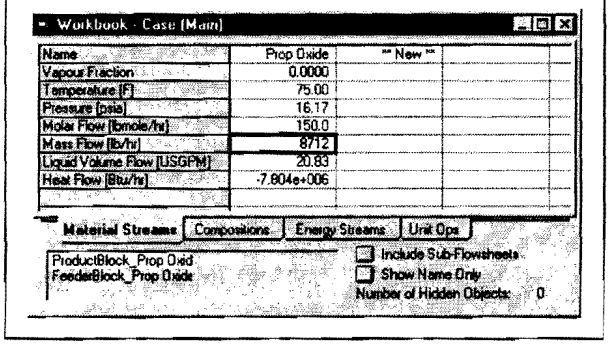


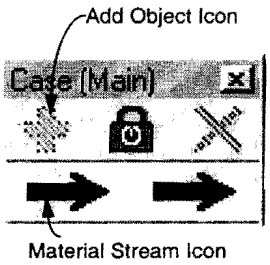
17. Click the **OK** button. HYSYS accepts the composition. The stream specification is now complete, so HYSYS will flash it at the conditions given to determine the remaining properties.

If you want to delete a stream, click on the Name cell for the stream, then press **DELETE**. HYSYS asks for confirmation of your action.

The values you specified are a different colour (blue) than the calculated values (black).

Figure 3.38





Adding Another Stream

Next, you will use an alternative method for adding a stream.

18. To add the second feed stream, do any **one** of the following:
    - Press **F11**.
    - From the **Flowsheet** menu, select **Add Stream**.
    - Double-click the **Material Stream** icon on the Object Palette.
    - Click the **Material Stream** icon on the Object Palette, then click the Palette's **Add Object** button.

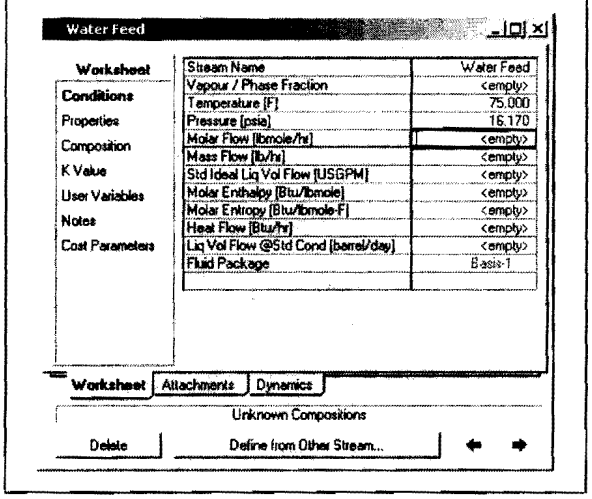
A new stream appears in the Workbook and is named according to the Auto Naming setting in your Session Preferences settings. The default setting names new material streams with numbers, starting at 1 (and energy streams starting at Q-100).

When you create the new stream, the stream's property view also appears, displaying the **Conditions** page of the **Worksheet** tab.

19. In the **Stream Name** cell, change the name to Water Feed.
20. In the **Temperature** cell, enter 75°F.
21. In the **Pressure** cell, enter 16.17 psia.

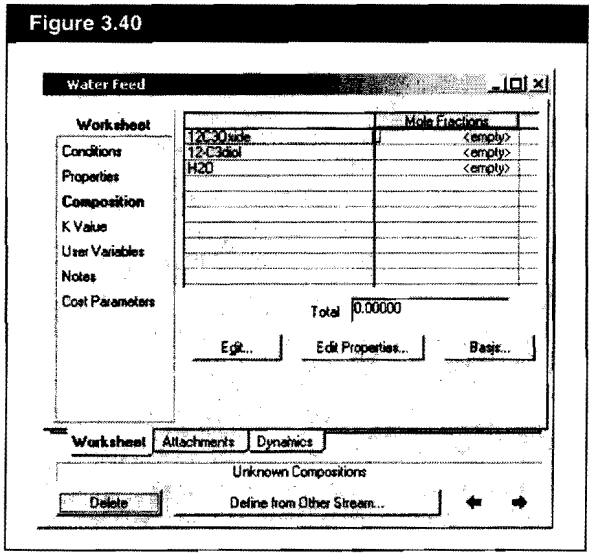
These parameters are in default units, so there is no need to change the units.

Figure 3.39



22. Select the **Composition** page to enter the compositional input for the new feed stream.

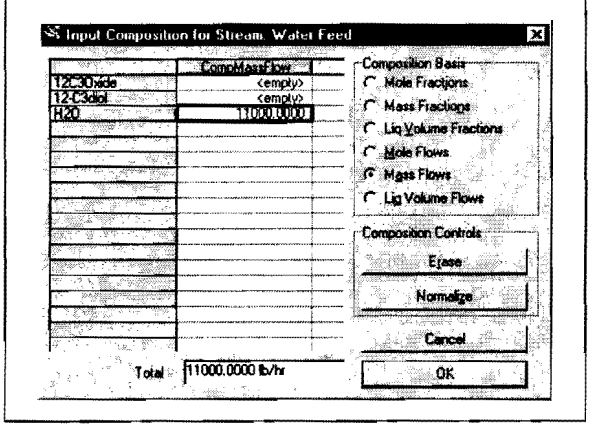
Figure 3.40



For the current Composition Basis setting, you want to enter the stream composition on a mass flow basis.

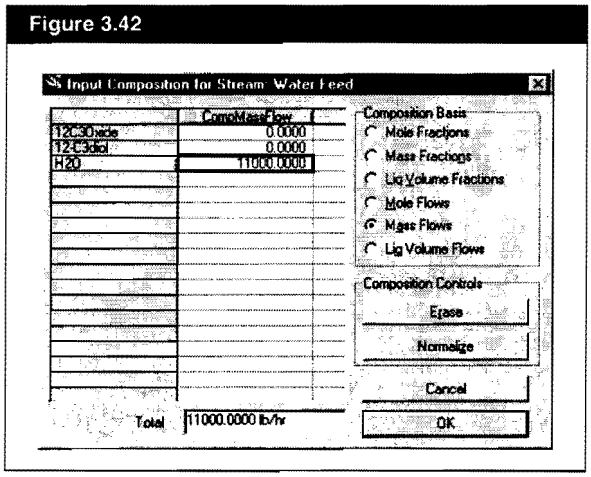
23. Click the **Edit** button near the bottom of the Composition page. The Input Composition for Stream view appears.
24. In the Composition Basis group, change the basis to **Mass Flows** by selecting the appropriate radio button, or by pressing ALT A.
25. In the **CompMassFlow** cell for H2O, type 11,000 (lb/hr), then press ENTER.

Figure 3.41



26. Since this stream has no other components, click the **Normalize** button. The other component mass flows are forced to zero.

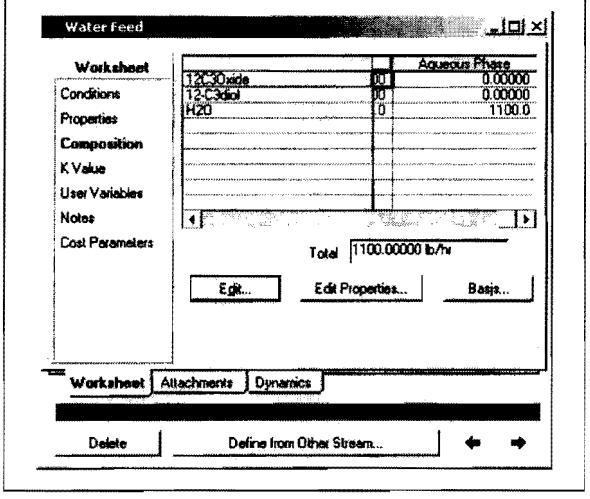
Figure 3.42



27. Click the **OK** button to close the view and return to the stream property view.

HYSYS performs a flash calculation to determine the unknown properties of Water Feed, and the status bar displays a green OK message. Use the horizontal scroll bar in the table to view the compositions of each phase.

Figure 3.43



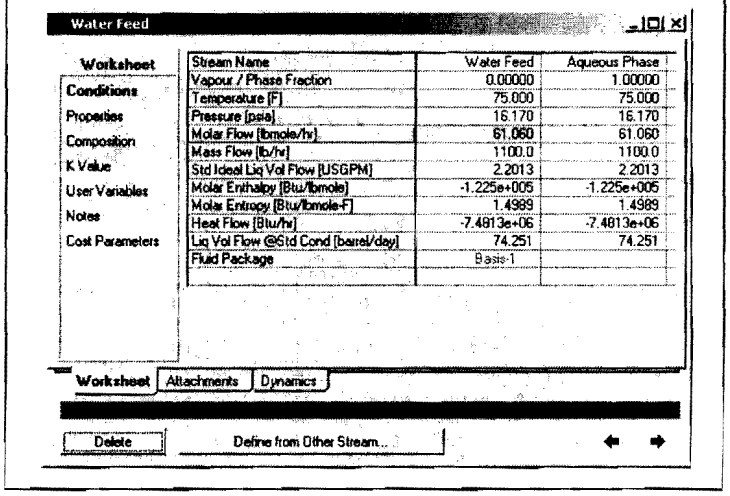
The compositions currently appear in Mass Flow, but you can change this by clicking the Basis button and choosing another Composition Basis radio button.

28. Click the **Conditions** page to view the calculated stream properties. You can display the properties of all phases by resizing the property view

Sizing Arrow Icon

29. Place the cursor over the right border of the view. The cursor changes to a double-ended sizing arrow.
30. With the sizing arrow visible, click and drag to the right until the horizontal scroll bar disappears, making the entire table visible.

Figure 3.44



New or updated information is automatically and instantly transferred among all locations in HYSYS.

In this case, the aqueous phase is identical to the overall phase.

31. Close the Water Feed property view to return to the Workbook.

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. As with most commands in HYSYS, installing an operation can be accomplished in a number of ways. One method is through the Unit Ops tab of the Workbook.

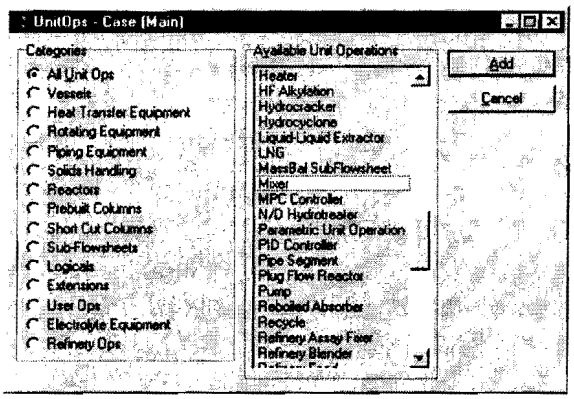
1. Click the **Workbook** icon to ensure the Workbook is active.
2. Click the **Unit Ops** tab of the Workbook.
3. Click the **Add UnitOp** button. The UnitOps view appears, listing all available unit operations.
   When you click the **Add** button or press ENTER inside this view, HYSYS adds the operation that is currently selected.
4. Select Mixer by doing **one** of the following:
   - Start typing 'mixer'.
   - Scroll down the list using the vertical scroll bar, then select Mixer.

Workbook Icon

You can also filter the list by selecting the Piping Equipment radio button in the Categories group, then use one of the above methods to install the operation.

Double-clicking on a listed operation can also be used instead of the Add button or the ENTER key.

Figure 3.45

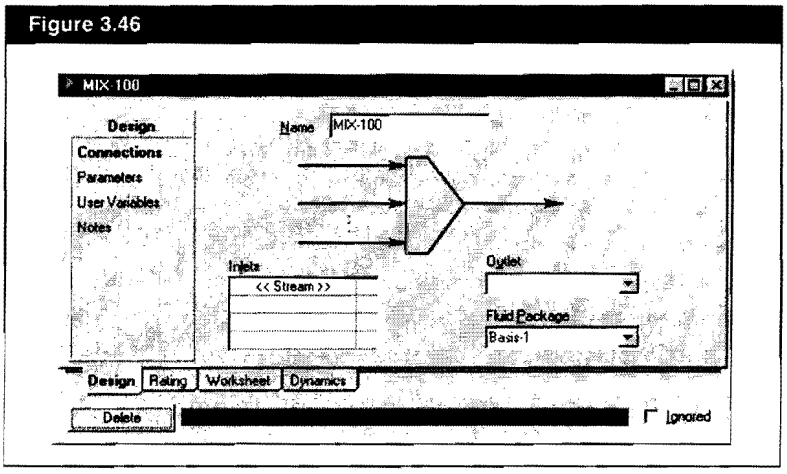


5. With Mixer selected, click the **Add** button, or press ENTER.

The property view for the Mixer appears.

The default naming scheme for unit operations can be changed in your Session Preferences.

Figure 3.46



The unit operation property view contains all the information required to define the operation, organized into tabs and pages. The Design, Rating, Worksheet and Dynamics tabs appear in the property view for most operations. Property views for more complex operations contain more tabs. HYSYS has provided the default name MIX-100 for the Mixer.

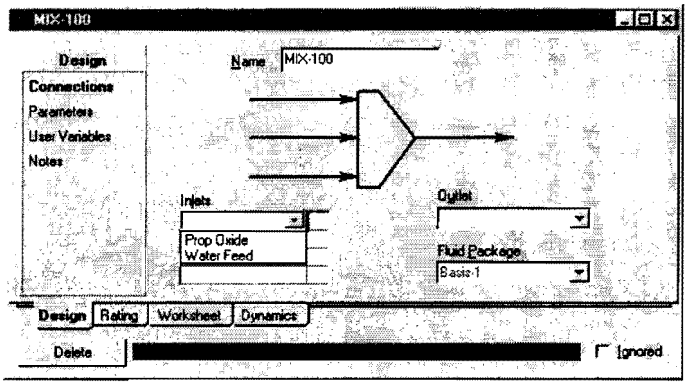
Many operations, like the Mixer, accept multiple feed streams. Whenever you see a table like the one in the Inlets group, the operation will accept multiple stream connections at that location. When the Inlets table is active, you can access a drop-down list of available streams.

Next, you will complete the Connections page for the Mixer.

6. In the Inlets table, click in the **<<Stream>>** cell. The status indicator at the bottom of the view indicates that the operation needs a feed stream.

7. Open the drop-down list of inlets by clicking on ↵ or by pressing the F2 key then SPACEBAR.

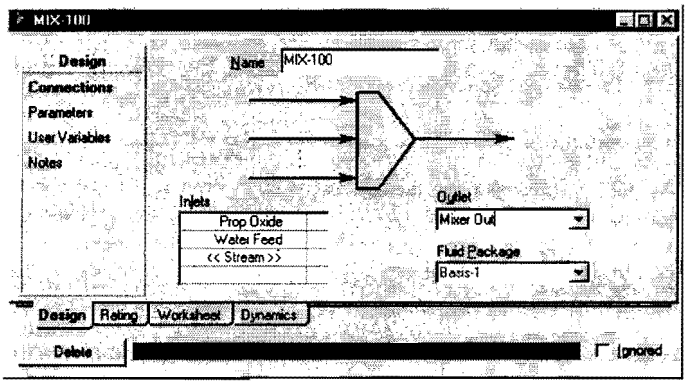
Figure 3.47



Alternatively, you can connect the stream by typing the exact stream name in the <<Stream>> cell, then pressing ENTER.

8. Select Prop Oxide from the drop-down list. The Prop Oxide stream appears in the Inlets table, and <<Stream>> automatically moves down to a new empty cell.
9. In the Inlets table, click the new empty **<<Stream>>** cell and select Water Feed from the list. The status indicator now displays 'Requires a product stream'.
10. Move to the **Outlet** field by pressing TAB, or by clicking in the cell.
11. Type Mixer Out in the cell, then press ENTER. HYSYS recognizes that there is no existing stream with this name, so it creates the new stream.

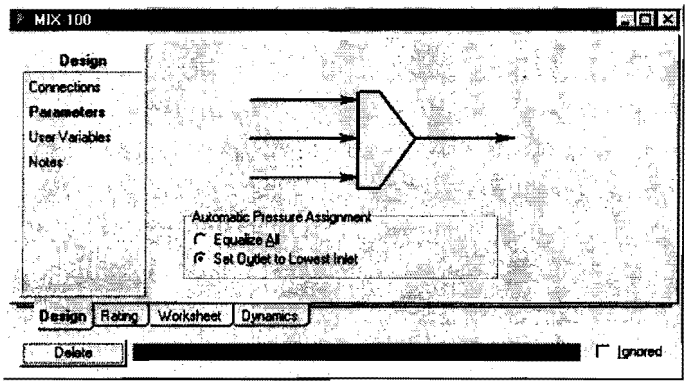
Figure 3.48



The status indicator displays a green **OK**, indicating that the operation and attached streams are completely calculated. The Connections page is now complete.

12. Click the **Parameters** page.
13. In the Automatic Pressure Assignment group, keep the default setting of **Set Outlet to Lowest Inlet**.

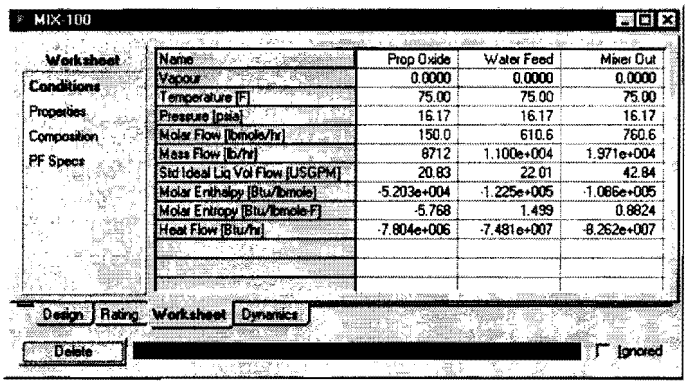
Figure 3.49



14. Click the **Worksheet** tab in the MIX-100 property view to view the calculated outlet stream. This tab is a condensed Workbook tab displaying only those streams attached to the operation.

HYSYS has calculated the outlet stream by combining the two inlets and flashing the mixture at the lowest pressure of the inlet streams. In this case, both inlets have the same pressure (16.17 psia), so the outlet stream is set to 16.17 psia.

Figure 3.50

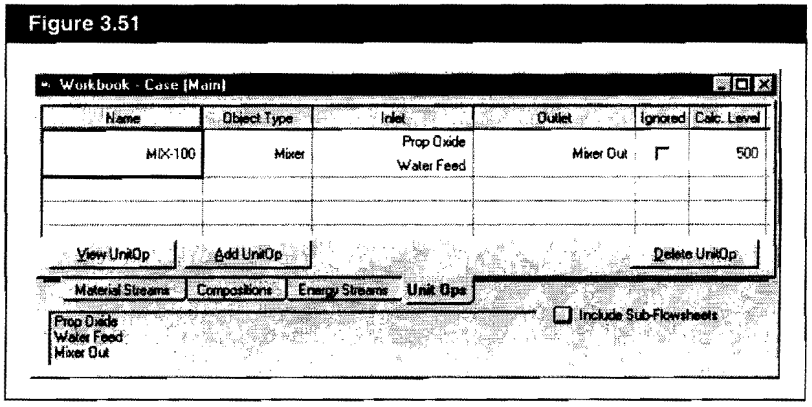


Name	Prop Oxide	Water Feed	Mixer Out
Vapour	0.0000	0.0000	0.0000
Temperature [F]	75.00	75.00	75.00
Pressure [psia]	16.17	16.17	16.17
Molar Flow [lbmole/hr]	150.0	610.6	760.6
Mass Flow [lb/hr]	8712	1.100e+004	1.971e+004
Std Ideal Liq Vol Flow [USGPM]	20.83	22.01	42.84
Molar Enthalpy [Btu/lbmole]	-5.203e+004	-1.225e+005	-1.086e+005
Molar Entropy [Btu/lbmole-F]	-5.768	1.499	0.8824
Heat Flow [Btu/hr]	-7.804e+006	-7.481e+007	-8.262e+007

15. Close the MIX-100 property view to return to the Workbook.

16. In the Workbook, click the **Unit Ops** tab. The new operation appears in the table.

Figure 3.51



The table shows the operation Name, Object Type, the attached streams (Inlet and Outlet), whether it is Ignored, and its Calc. Level. When you click the View UnitOp button, the property view for the currently selected operation appears. Alternatively, by double-clicking on any cell (except Inlet or Outlet) associated with the operation, you will also open its property view.

You can also open a stream property view directly from the Workbook Unit Ops tab. When any of the cells Name, Object Type, Ignored or Calc. Level are selected, the gray box at the bottom of the view displays all streams attached to the current operation. Currently, the Name cell for MIX-100 has focus, so the box displays the three streams attached to this operation.

For example, to open the property view for the Prop Oxide stream attached to the Mixer, do **one** of the following:

- Double-click on Prop Oxide in the box at the bottom of the view.
- Double-click on the Inlets cell for MIX-100. The property view for the first listed feed stream, in this case Prop Oxide, appears.

Workbook Features

Before installing the remaining operations, you will examine a number of Workbook features that allow you to access information quickly and change how information is displayed.

Accessing Unit Operations from the Workbook

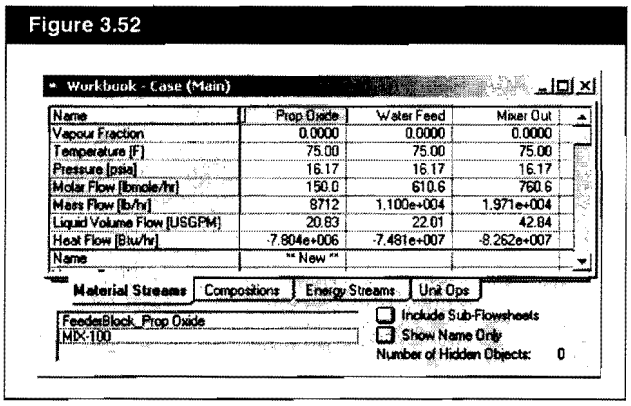
While you can easily access the property view for a unit operation from the Unit Ops tab of the Workbook, you can also access operations from the Material Streams, Compositions, and Energy Streams tabs.

Any utilities attached to the stream with focus in the Workbook are also displayed in (and are accessible from) this box.

When your current location is a Workbook streams tab, the gray box at the bottom of the Workbook view displays the operations to which the current stream is attached. For example, click on any cell associated with the stream Prop Oxide. The gray box displays the name of the mixer operation, MIX-100.

If the stream Prop Oxide was also attached to another unit operation, both unit operations would be listed in the box. To access the property view for the Mixer, double-click on its name in the gray box.

Figure 3.52



Adding a Tab to the Workbook

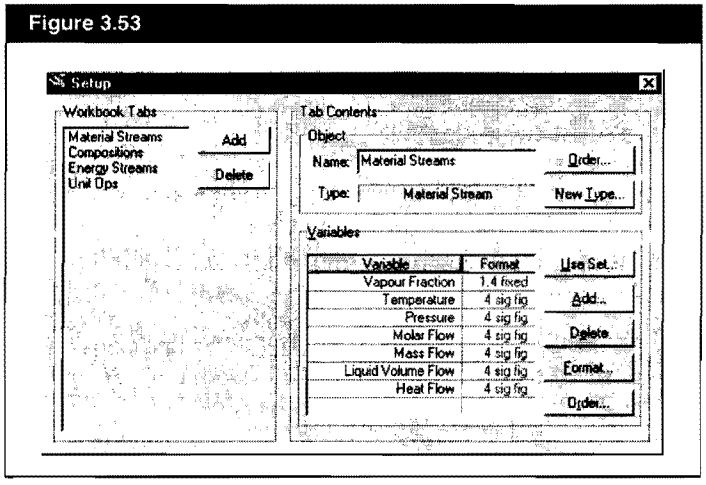
When the Workbook is active, the Workbook item appears in the HYSYS menu bar. This item allows you to customize the Workbook.

Next you will create a new Workbook tab that displays only stream pressure, temperature, and flow.

1. Do one of the following:
   - From the Workbook menu item, select **Setup**.
   - Object inspect (right-click) the **Material Streams** tab in the Workbook, then select **Setup** from the menu that appears.

The Workbook Setup view appears.

Figure 3.53

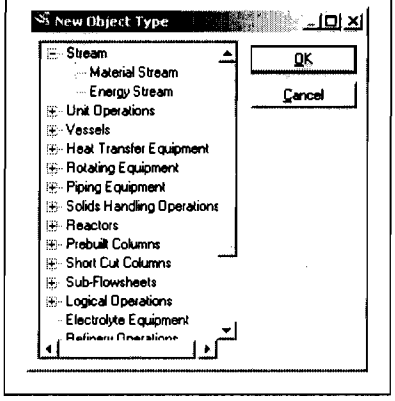


The four existing tabs are listed in the Workbook Tabs area. When you add a new tab, it will be inserted before the highlighted tab (currently Material Streams). You will insert the new tab between the Materials Streams tab and the Compositions tab.

2. In the Workbook Tabs list, select Compositions, then click the **Add** button. The New Object Type view appears.

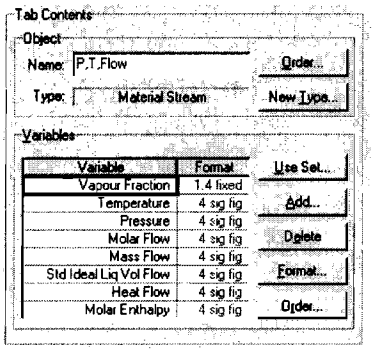
3. Click the + beside Stream to expand the tree.

Figure 3.54



4. Select Material Stream, then click the **OK** button. You return to the Setup view, and the new tab Material Streams 1 appears after the existing Material Streams tab.
5. In the Object group, click in the **Name** field and change the name for the new tab to P,T,Flow to better describe the tab contents.

Figure 3.55

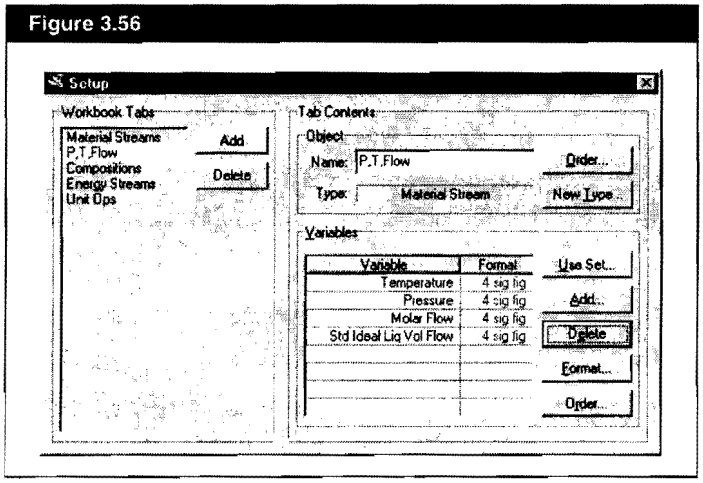


The next task is to customize the tab by removing the variables that are irrelevant.

6. In the Variables table, select the first variable, Vapour Fraction.
7. Press and hold the CTRL key.
8. Select the following variables: Mass Flow, Heat Flow, and Molar Enthalpy.
9. Release the CTRL key.
10. Click the **Delete** button beside the table to remove the selected variables from this Workbook tab only. The finished Setup appears in the figure below.

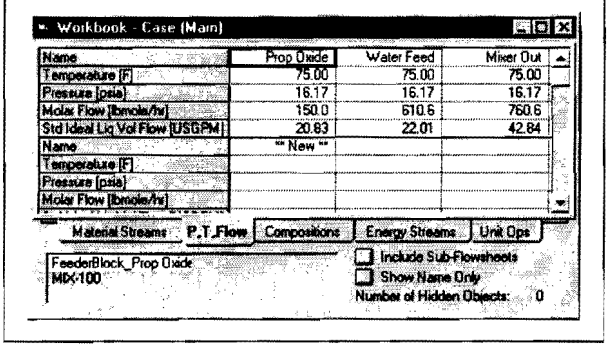
If you want to remove variables from another tab, you must edit each tab individually.

Figure 3.56



11. Close the Setup view. The new tab appears in the Workbook.

Figure 3.57



12. Save the case.

3.2.7 Installing Equipment on the PFD

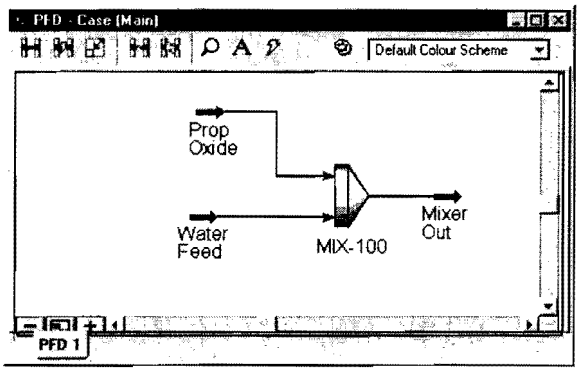
PFD Icon

Besides the Workbook, the PFD is the other main view in HYSYS you will use to build the simulation.

To open the PFD, click the PFD icon on the toolbar. The PFD item appears in the HYSYS menu bar whenever the PFD has focus.

When you open the PFD view, it appears similar to the one shown below.

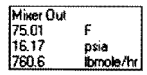
Figure 3.58



Like any other non-modal view, the PFD view can be re-sized by clicking and dragging anywhere on the outside border.

As a graphical representation of your flowsheet, the PFD shows the connections among all streams and operations, also known as "objects". Each object is represented by a symbol, also known as an "icon". A stream icon is an arrow pointing in the direction of flow, while an operation icon is a graphic representing the actual physical operation. The object name, also known as a "label", appears near each icon.

The PFD shown above has been rearranged by moving the Prop Oxide feed stream icon up slightly so it does not overlap the Water Feed stream icon. To move an icon, simply click and drag it to a new location. You can click and drag either the icon (arrow) itself, or the label (stream name), as these two items are grouped together.



Fly-by information

Size Icon

Zoom Out 25%

Display Entire PFD

Zoom In 25%

Other functions that can be performed while the PFD is active include the following:

- Access commands and features through the PFD tool bar.
- Open the property view for an object by double-clicking its icon.
- Move an object by clicking and dragging it to the new location.
- Access "fly-by" summary information for an object by placing the cursor over it.
- Size an object by clicking the Size icon, selecting the object, then clicking and dragging the sizing "handles" that appear.
- Display the Object Inspection menu for an object by placing the cursor over it and right-clicking. This menu provides access to a number of commands associated with the particular object.
- Zoom in and out, or display the entire flowsheet in the PFD window by clicking the zoom buttons at the bottom left of the PFD view.

Some of these functions will be illustrated in this tutorial; for more information, refer to the **User Guide**.

Calculation Status

HYSYS uses colour-coding to indicate calculation status for objects, both in the object property views, and in the flowsheet. If you recall, the status bar indicator at the bottom of a property view for a stream or operation indicates the current state of the object:

These are the HYSYS default colours; you may change the colours in the Session Preferences.

Indicator Status	Description
Red Status	A major piece of defining information is missing from the object. For example, a feed or product stream is not attached to a Separator. The status indicator is red, and an appropriate warning message is displayed.
Yellow Status	All major defining information is present, but the stream or operation has not been solved because one or more degrees of freedom is present. For example, a Cooler whose outlet stream temperature is unknown. The status indicator is yellow, and an appropriate warning message is displayed.
Green Status	The stream or operation is completely defined and solved. The status indicator is green, and an **OK** message is displayed.

When you are in the PFD, the streams and operations are colour-coded to indicate their calculation status. If the conditions of an attached stream for an operation were not entirely known, the operation would have a yellow outline indicating its current status. For the Mixer, all streams are defined, so it has no yellow outline.

Notice that the icons for all streams installed to this point are dark blue.

Another colour scheme is used to indicate the status of streams. For material streams, a dark blue icon indicates the stream has been flashed and is entirely known. A light blue icon indicates the stream cannot be flashed until some additional information is supplied. Similarly, a dark red icon is for an energy stream with a known duty, while a purple icon indicates an unknown duty.

Installing the Reactor

Next, you will install a continuously-stirred-tank reactor operation (CSTR). You can install streams or operations by dropping them from the Object Palette onto the PFD.

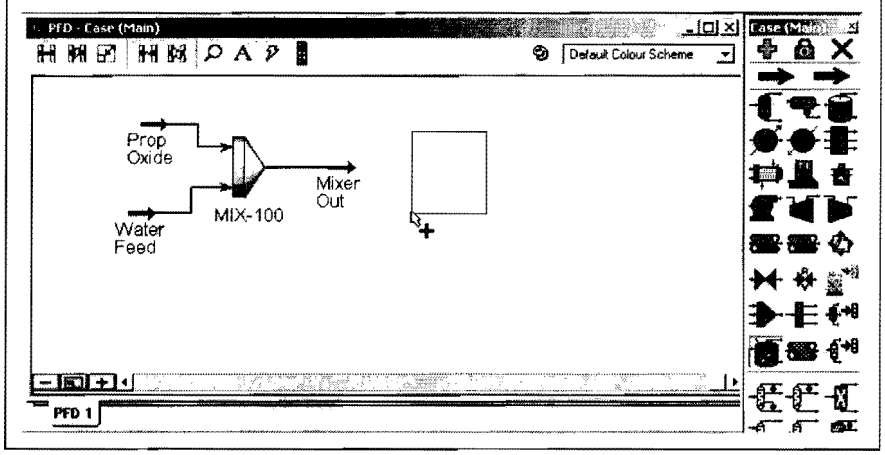
1. Ensure that the Object Palette is displayed; if it is not, press F4.
2. You will add the CSTR to the right of the Mixer, so if you need to make some empty space available in the PFD, scroll to the right using the horizontal scroll bar.
3. In the Object Palette, click the CSTR icon.

CSTR Icon

4. Position the cursor in the PFD to the right of the Mixer Out stream. The cursor changes to a special cursor with a plus (+) symbol attached to it. The symbol indicates the location of the operation icon.

Cancel Icon

Figure 3.59



5. Click to "drop" the Reactor onto the PFD. HYSYS creates a new Reactor with a default name, CSTR-100. The Reactor has red status (colour), indicating that it requires feed and product streams.

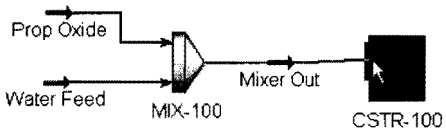
Attaching Streams to the Reactor

Attach Mode Icon

When you are in Attach mode, you will not be able to move objects in the PFD. To return to Move mode, click the Attach button again. You can temporarily toggle between Attach and Move mode by holding down the CTRL key.

1. Click the **Attach Mode** icon on the PFD toolbar to enter Attach mode. The Attach Mode button stays active until you click it again.
2. Position the cursor over the right end of the Mixer Out stream icon. A small white box appears at the cursor tip with a pop-up description 'Out', indicating that the stream outlet is available for connection.

Figure 3.60

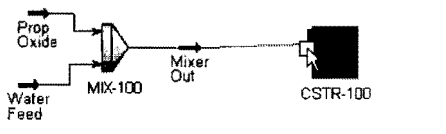


3. With the pop-up 'Out' visible, click and hold the mouse button. The transparent box becomes solid black, indicating that you are beginning a connection.

Multiple connection points appear because the Reactor accepts multiple feed streams.

4. Move the cursor toward the left (inlet) side of the CSTR-100 icon. A line appears between the Mixer Out stream icon and the cursor, and multiple connection points (blue) appear at the Reactor inlet.
5. Place the cursor near a connection point until a solid white box appears at the cursor tip, indicating an acceptable end point for the connection.

Figure 3.61

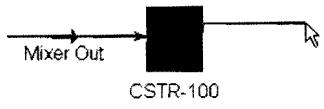


6. Release the mouse button, and the connection is made between the stream and the CSTR-100 inlet.
7. Position the cursor over top right-hand corner of the CSTR-100 icon. The white box and the pop-up 'Vapour Product' appear.
8. With the pop-up visible, left-click and hold. The white box again becomes solid black.

Break Connection Icon

9. Move the cursor to the right of the CSTR-100. A stream icon appears with a trailing line attached to the CSTR-100 outlet. The stream icon indicates that a new stream will be created when you complete the next step.

Figure 3.62



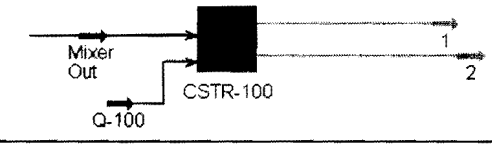
10. With the stream icon visible, release the left mouse button. HYSYS creates a new stream with the default name 1.
11. Place the cursor over the bottom right connection point on the reactor labeled 'Liquid Product', then click and drag to the right to create the reactor's liquid product stream. The new stream is given the default name 2.
12. Place the cursor over the bottom left connection point on the reactor labeled 'Energy Stream', then click and drag down and to the left to create the reactors energy stream. The new stream is automatically named Q-100.

If you make an incorrect connection, break the connection and try again.

1. Click the **Break Connection** icon on the PFD tool bar.
2. Place the cursor over the stream line you want to break. The cursor shows a checkmark, indicating an available connection to break.
3. Click once to break the connection.

The reactor displays a yellow warning status, indicating that all necessary connections have been made, but that the attached streams are not entirely known.

Figure 3.63



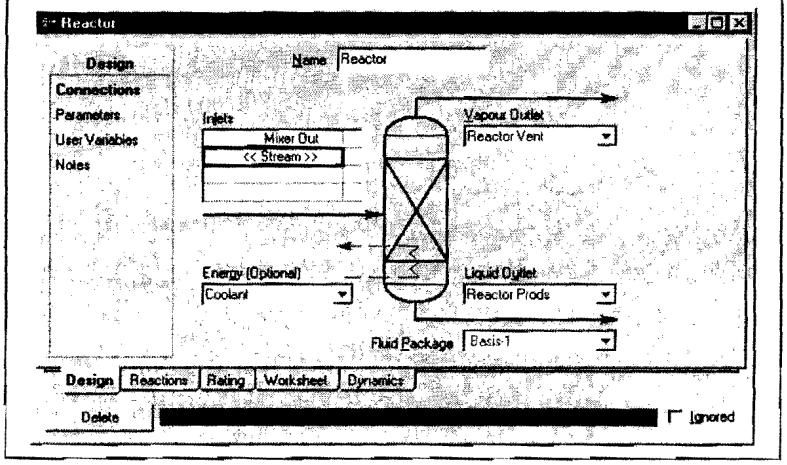
13. Click the **Attach Mode** icon again to return to Move mode.
14. Double-click the steam icon 1 to open its property view.
15. In the **Stream Name** cell, enter the new name Reactor Vent, then close the property view.
16. Double-click the stream 2 icon. Rename this stream Reactor Prods, then close the property view.
17. Double-click the Q-100 icon, rename it Coolant, then close the view.

The reactor outlet and energy streams are unknown at this point, so they are light blue and purple, respectively.

Completing the Reactor Specifications

1. Double-click the CSTR-100 icon to open its property view.
2. Click the Design tab, then select the Connections page (if required). The names of the Inlet, Outlet and Energy streams that were attached before appear in the appropriate cells.
3. In the **Name** cell, change the operation name to Reactor.

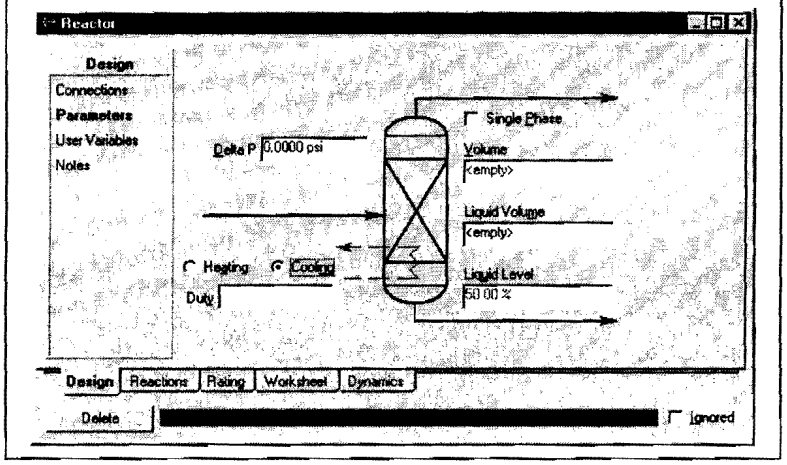
Figure 3.64



4. Select the **Parameters** page. For now, the **Delta P** and the **Volume parameters** are acceptable at the default values.

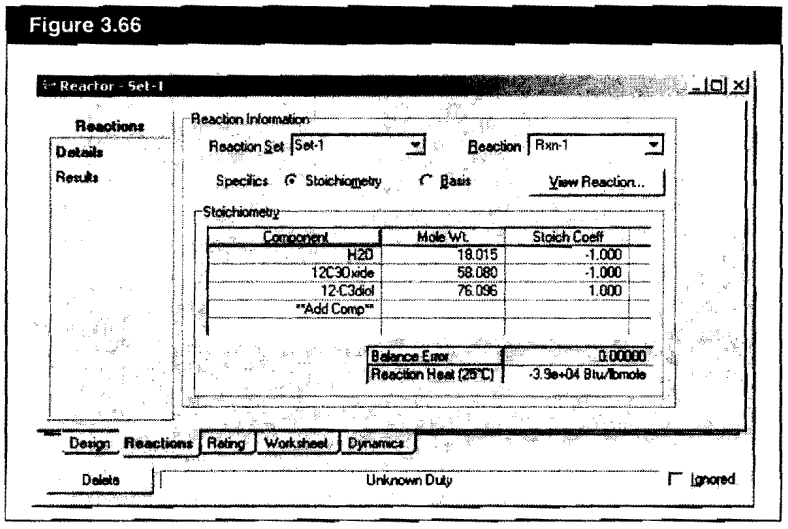
5. Select the **Cooling** radio button. This reaction is exothermic (produces heat), so cooling is required.

Figure 3.65



6. Click the **Reactions** tab. Next you will attach the Reaction Set that you created in the Basis Environment.
7. From the Reaction Set drop-down list, select Set-1. The completed **Reactions** tab appears below.

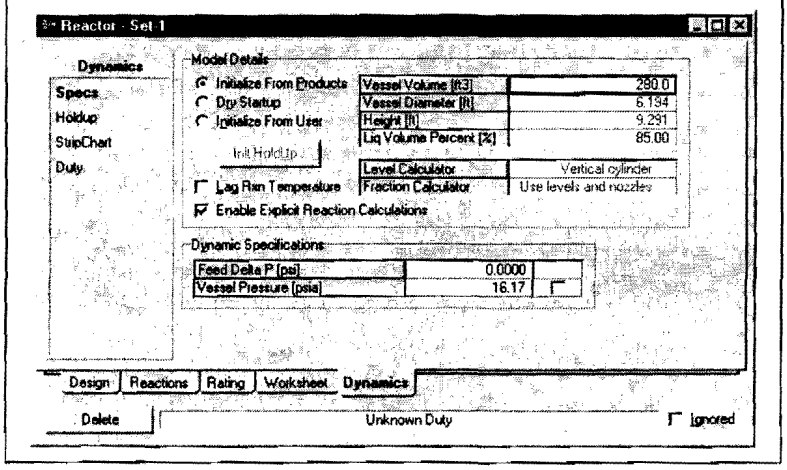
Figure 3.66



The next task is to specify the Vessel Parameters. In this Tutorial, the reactor has a volume of 280 ft3 and is 85% full.

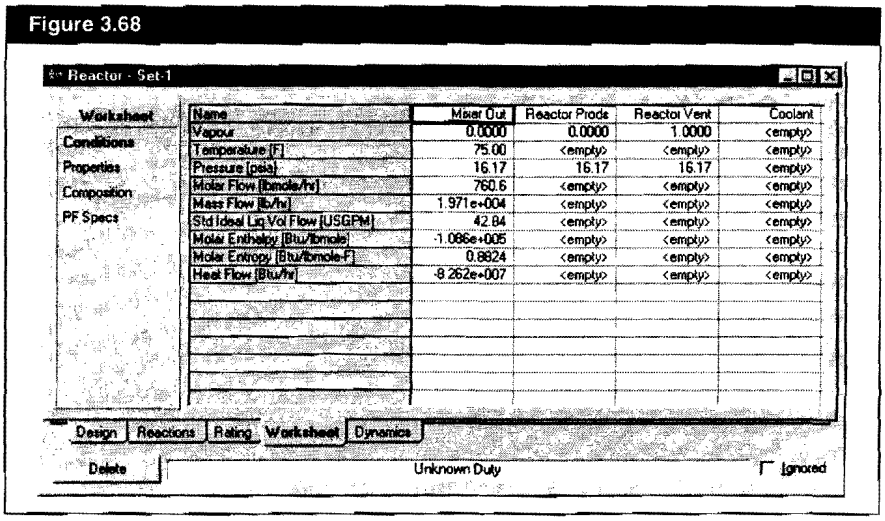
8. Click the **Dynamics** tab, then select the **Specs** page.
9. In the Model Details group, click in the **Vessel Volume** cell. Type 280 (ft3), then press ENTER.
10. In the **Liq Volume Percent** cell, type 85, then press ENTER. HYSYS automatically calculates the Liquid Volume in the vessel (280 ft3 x 85% full = 238 ft3), displayed on the Parameters page of the Design tab.

Figure 3.67



11. Click on the **Worksheet** tab.

Figure 3.68

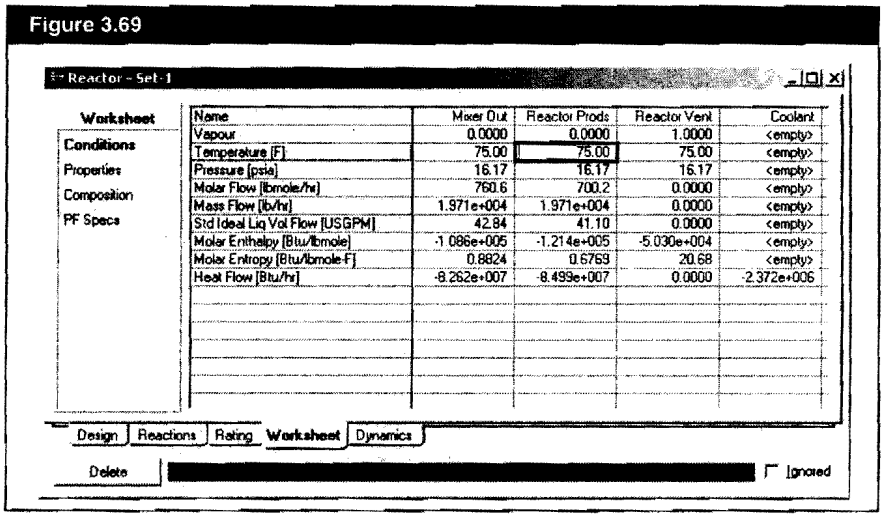


At this point, the Reactor product streams and the energy stream Coolant are unknown because the Reactor has one degree of freedom. At this point, either the outlet stream temperature or the cooling duty can be specified. For this example, you will specify the outlet temperature.

Initially the Reactor is assumed to be operating at isothermal conditions, therefore the outlet temperature is equivalent to the feed temperature, 75°F.

12. In the Reactor Prods column, click in the **Temperature** cell. Type 75, then press ENTER. HYSYS solves the Reactor.

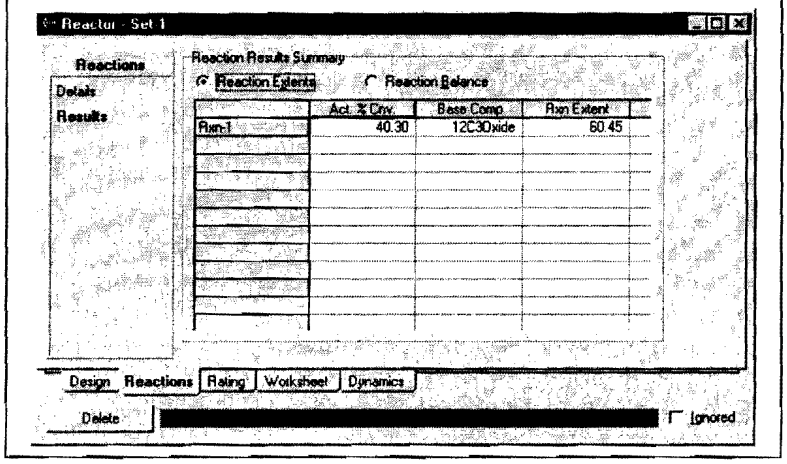
Figure 3.69



There is no phase change in the Reactor under isothermal conditions since the flow of the vapour product stream Reactor Vent is zero. In addition, the required cooling duty has been calculated and is represented by the Heat Flow of stream Coolant. The next step is to examine the Reactor conversion as a function of temperature.

13. Click the **Reactions** tab, then select the **Results** page. The conversion appears in the Reactor Results Summary table.

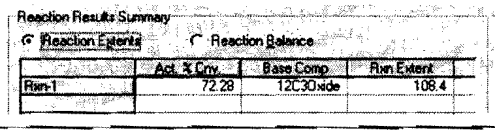
Figure 3.70



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

14. Click the **Worksheet** tab.
15. In the Reactor Prods column, change the **Temperature** to 100°F.
16. Return to the **Reactions** tab to check the conversion, which has increased to 72.28% as shown below.

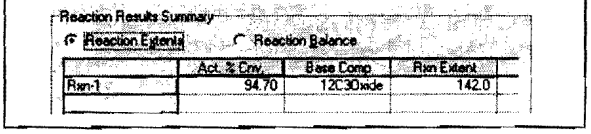
Figure 3.71



17. Return to the **Worksheet** tab, and change the **Temperature** of Reactor Prods to 140°F.

18. Click the **Reactions** tab again and check the conversion. The conversion at 140°F is approximately 95%, which is acceptable.

Figure 3.72



19. Close the Reactor property view.

Installing the Column

HYSYS has a number of pre-built column templates that you can install and customize by changing attached stream names, number of stages and default specifications. For this example, a Distillation Column will be installed.

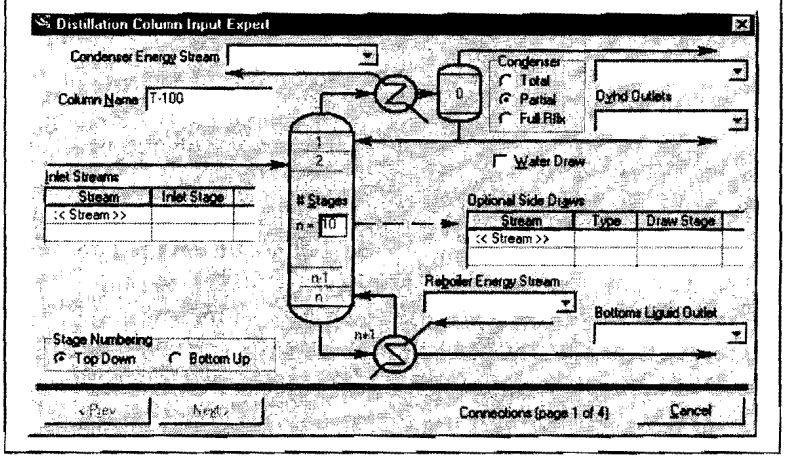
1. Before installing the column, click the **Tools** menu and select **Preferences**. On the **Simulation** tab, click on the **Options** page and ensure that the **Use Input Experts** checkbox is selected (checked), then close the view.
2. Double-click the **Distillation Column** icon on the Object Palette. The first page of the Input Expert appears.

Distillation Column Icon

The Input Expert is a logical sequence of input views that guide you through the initial installation of a Column. Complete the steps to ensure that you have provided the minimum amount of information required to define the column.

The Input Expert is a Modal view, indicated by the absence of the Maximize/Minimize icons. You cannot exit or move outside the Expert until you supply the necessary information, or click the **Cancel** button.

Figure 3.73



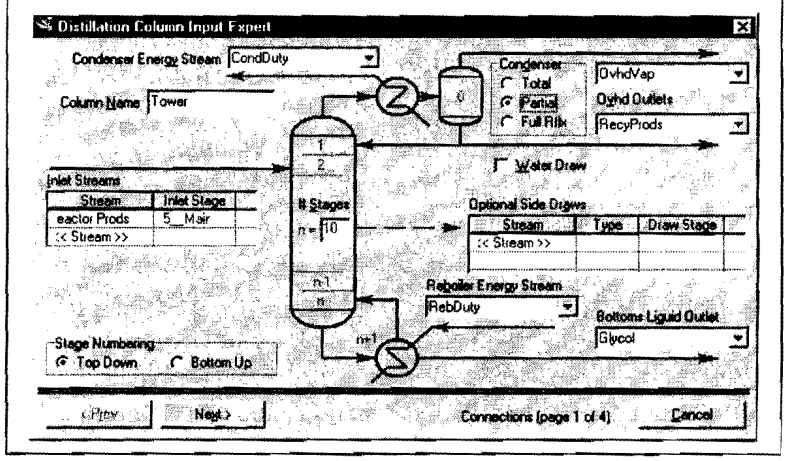
When you install a column using a pre-built template, HYSYS supplies certain default information, such as the number of stages. The **Numb of Stages** field contains **10** (default number of stages). Note the following:

- These are theoretical stages, as the HYSYS default stage efficiency is one.
- The Condenser and Reboiler are considered separate from the other stages, and are not included in the Num of Stages field.

3. For this example, 10 theoretical stages are used, so leave the **Numb of Stages** at its default value.
4. In the Inlet Streams table, click in the **<<Stream>>** cell.
5. From the drop-down list of available inlet streams, select **Reactor Prods** as the feed stream to the column. HYSYS supplies a default feed location in the middle of the Tray Section (TS), in this case stage 5 (indicated by 5_Main TS).
6. In the **Condenser** group, ensure the **Partial** radio button is selected, as the column will have both Vapour and Liquid Overhead Outlets.
7. In the **Column Name** field, change the name to Tower.
8. In the **Condenser Energy Stream** field, type CondDuty, then press ENTER.
9. In the top **Ovhd Outlets** field, type OvhdVap, then press ENTER. In the bottom **Ovhd Outlets** field, type RecyProds, then press ENTER.
10. In the **Reboiler Energy Stream** field, type RebDuty, then press ENTER.
11. In the **Bottoms Liquid Outlet** field, type Glycol, then press ENTER.

When you are finished, the Next button becomes active, indicating sufficient information has been supplied to advance to the next page of the Input Expert. The first page of the Input Expert should appear as shown in the following figure.

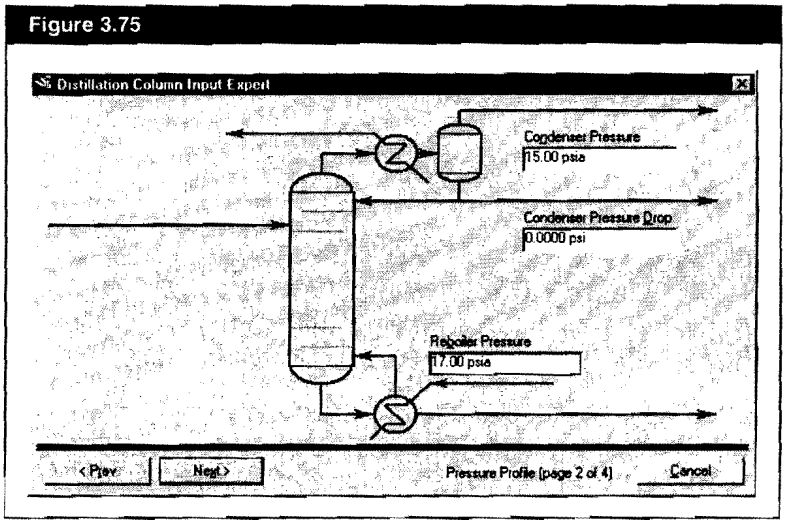
Figure 3.74



12. Click the **Next** button to advance to the **Pressure Profile** page.

13. In the **Condenser Pressure** field, enter 15 psia.
    In the **Reboiler Pressure** field, enter 17 psia.
    Leave the **Condenser Pressure Drop** at its default value of zero.

Figure 3.75



Although HYSYS does not require estimates to produce a converged column, you should provide estimates for columns that are difficult to converge.

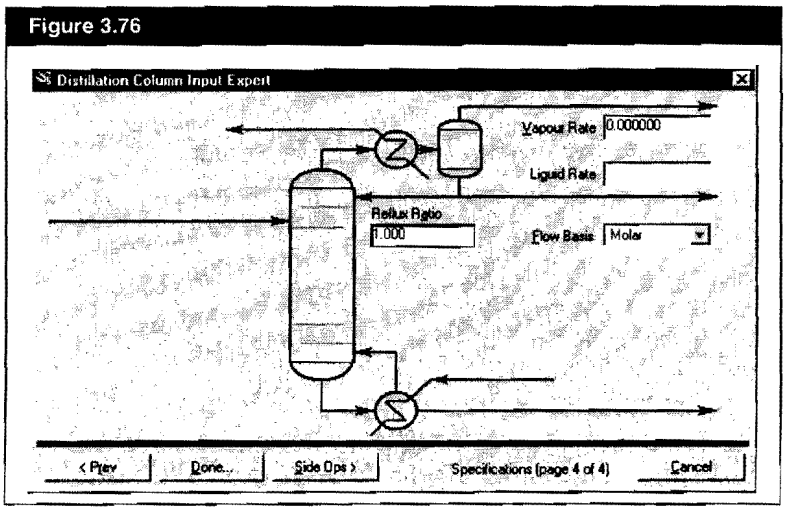
14. Click the **Next** button to advance to the **Optional Estimates** page. For this example, no estimates are required.
15. Click the **Next** button to advance to the fourth and final page of the Input Expert. This page allows you to supply values for the default column specifications that HYSYS has created.

In general, a Distillation Column has three default specifications. The overhead Vapour Rate and Reflux Ratio will be used as active specifications, and later you will create a glycol purity specification to exhaust the third degree of freedom. The third default specification, overhead Liquid Rate, will not be used.

The Flow Basis applies to the Vapour Rate, so leave it at the default of Molar.

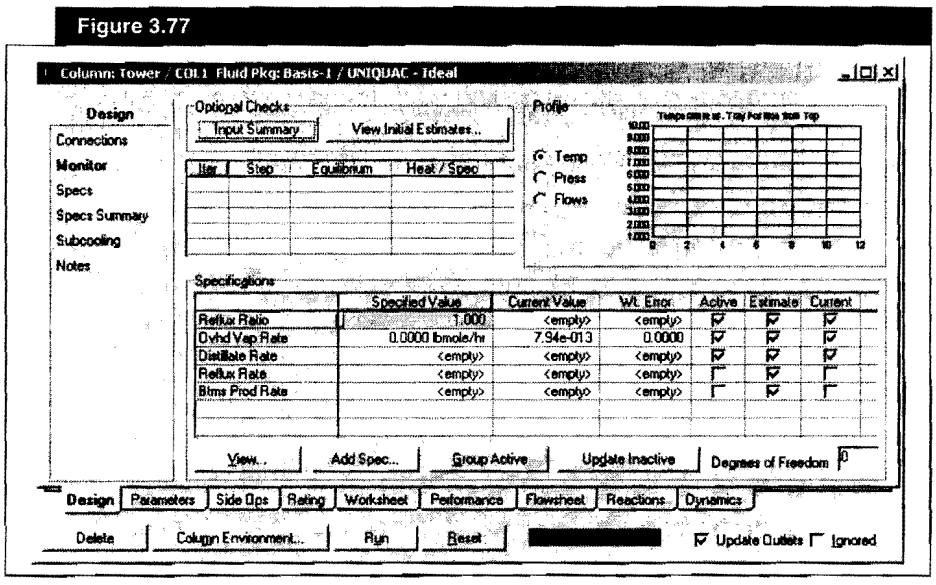
16. In the **Vapour Rate** field, enter 0 lbmole/hr.
    In the **Reflux Ratio** field, enter 1.0.

Figure 3.76



17. Click the **Done** button. The Column property view appears.
18. On the **Design** tab, select the **Monitor** page.

Figure 3.77

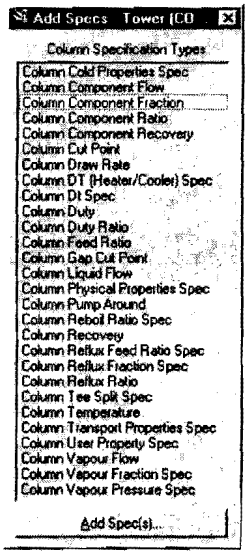


You can also change specification values, and activate or de-activate specifications used by the Column solver directly from the Monitor page.

The Monitor page displays the status of your column as it is being calculated, updating information with each iteration.

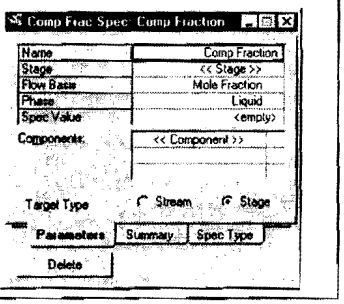
Adding a Column Specification

The current Degrees of Freedom is zero, indicating the column is ready to be run, however, the Distillate Rate (Overhead Liquid Rate for which no value was provided in the Input Expert) is currently an Active specification with a Specified Value of <empty>. For this example, you will specify a water mole fraction of 0.005 in the Glycol product stream.



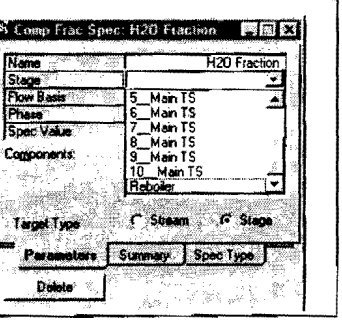
1. Since it is not desirable to use this specification, clear the **Active** checkbox for the Distillate Rate. The Degrees of Freedom increases to 1, indicating that another active specification is required.
2. On the **Design** tab, select the **Specs** page.
3. In the Column Specifications group, click the **Add** button. The Add Specs view appears.
4. Select Column Component Fraction as the Specification Type.
5. Click the **Add Spec(s)** button. The Comp Frac Spec view appears.

Figure 3.78



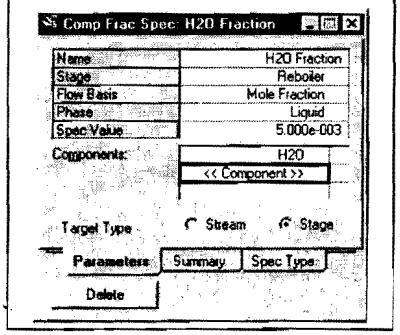
6. In the **Name** cell, change the name to H2O Fraction.
7. In the **Stage** cell, select Reboiler from the drop-down list.

Figure 3.79



8. In the **Spec Value** cell, enter 0.005 as the liquid mole fraction specification value.
9. In the Components list, click in the first cell labeled **<<Component>>**, then select H2O from the drop-down list of available components.

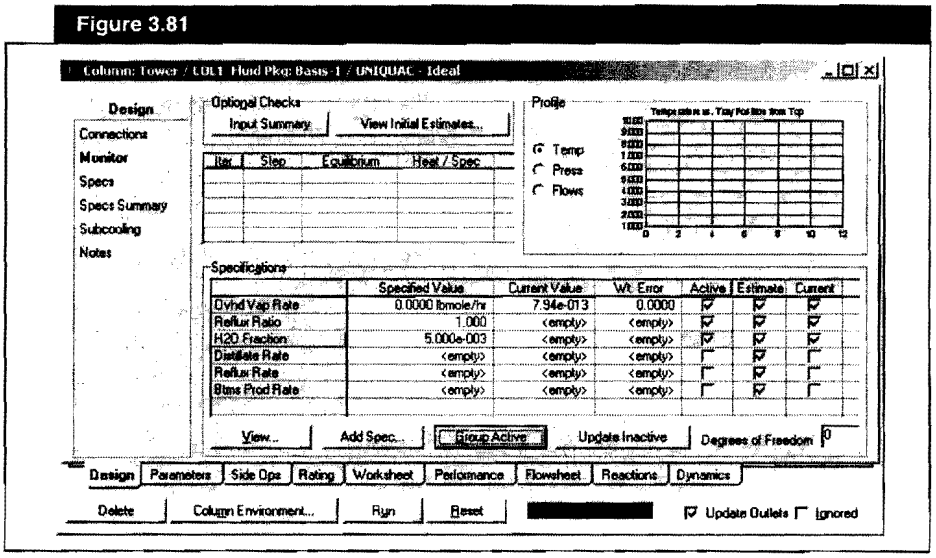
Figure 3.80



10. Close this view to return to the Column property view. The new specification appears in the Column Specifications list on the **Specs** page.
11. Return to the **Monitor** page, where the new specification appears at the bottom of the Specifications list.
12. Click the **Group Active** button to bring the new specification to the top of the list, directly under the other Active specifications.

If you want to view the entire Specifications table, re-size the view by clicking and dragging its bottom border.

Figure 3.81



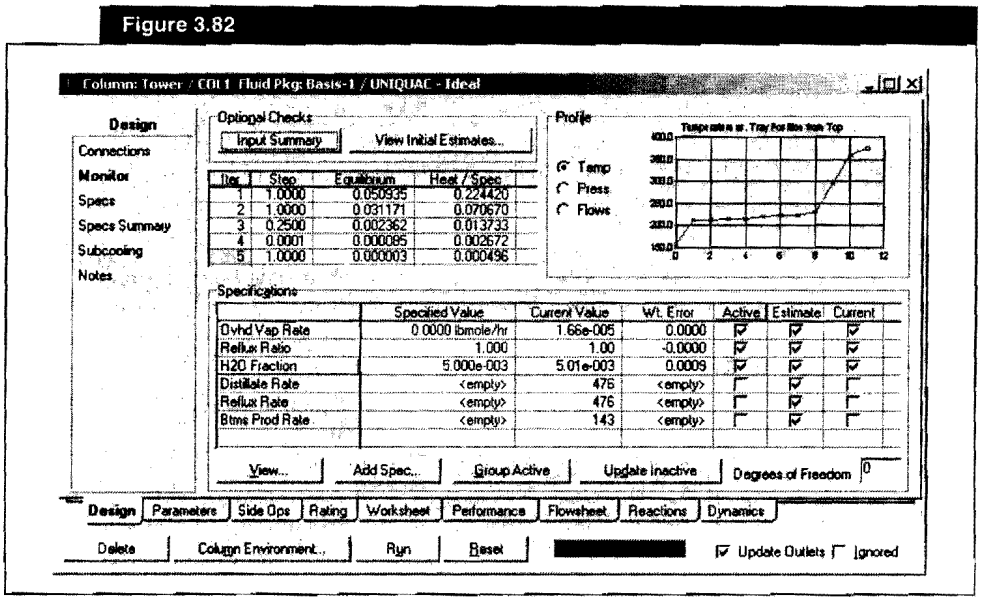
HYSYS automatically made the new specification Active when you created it.

The Degrees of Freedom has returned to zero, so the column is ready to be calculated.

Running the Column

1. Click the **Run** button to begin calculations, and the information displayed on the page is updated with each iteration. The column converges quickly, in five iterations.

Figure 3.82

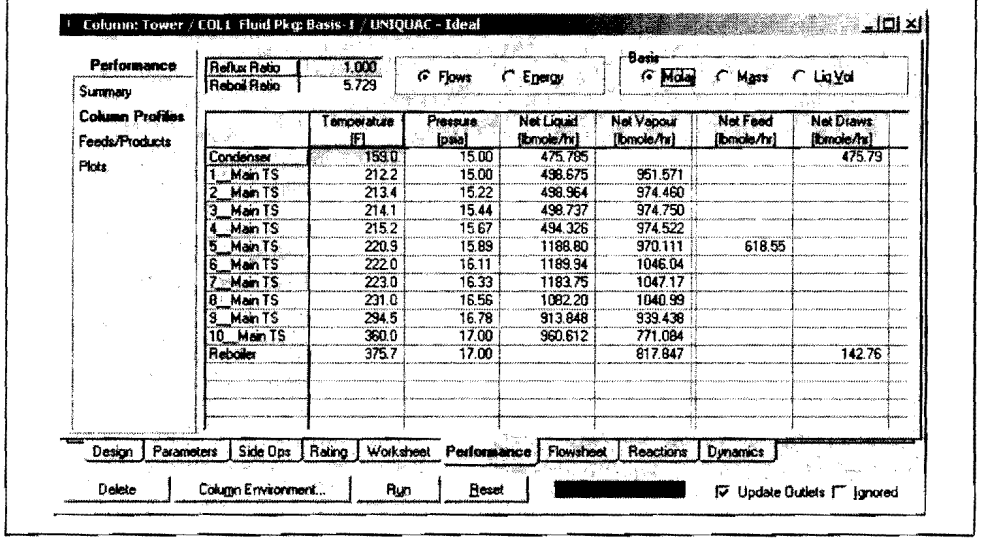


The converged temperature profile appears in the upper right corner of the view.

2. Select the **Press** or **Flow** radio button to view the pressure or flow profiles.

3. To access a more detailed stage summary, click the **Performance** tab, then select the **Column Profiles** page.

Figure 3.83



Accessing the Column Sub-flowsheet

When considering the column, you might want to focus only on the column sub-flowsheet. You can do this by entering the column environment.

PFD Icon

Workbook Icon

Column Runner Icon

1. Click the **Column Environment** button at the bottom of the property view. While inside the column environment, you can do the following:
   - View the column sub-flowsheet PFD by clicking the **PFD** icon.
   - View a Workbook of the column sub-flowsheet objects by clicking the **Workbook** icon.
   - Access the "inside" column property view by clicking the **Column Runner** icon. This property view is essentially the same as the "outside", or Main Flowsheet, property view of the column.

The column sub-flowsheet PFD and Workbook appear in the following figures.

Figure 3.84

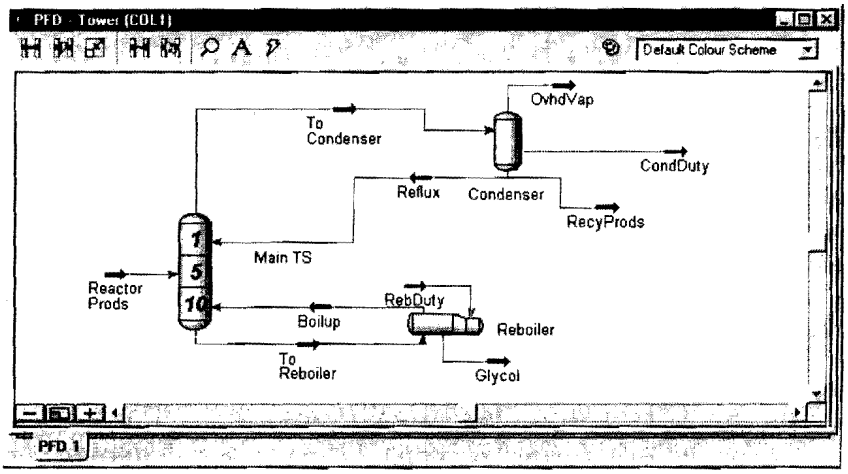
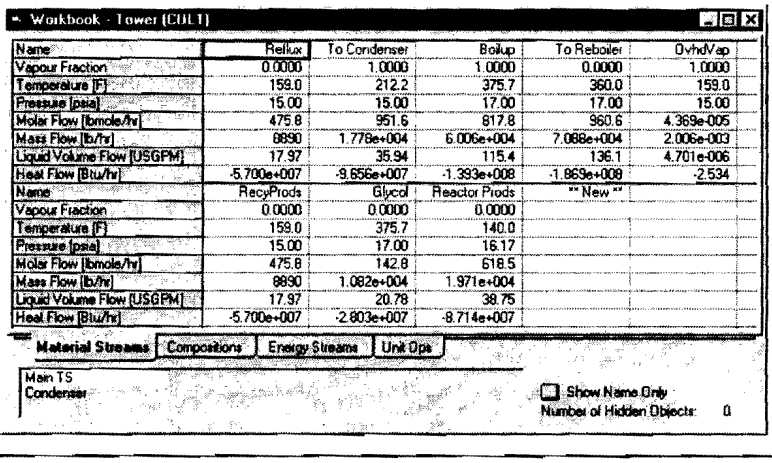


Figure 3.85



Name	Reflux	To Condenser	Boilup	To Reboiler	OvhdVap
Vapour Fraction	0.0000	1.0000	1.0000	0.0000	1.0000
Temperature [F]	159.0	212.2	375.7	360.0	159.0
Pressure [psia]	15.00	15.00	17.00	17.00	15.00
Molar Flow [lbmole/hr]	475.8	951.6	817.8	960.6	4.369e-005
Mass Flow [lb/hr]	9890	1.778e+004	6.006e+004	7.088e+004	2.006e-003
Liquid Volume Flow [USGPM]	17.97	35.94	115.4	136.1	4.701e-006
Heat Flow [Btu/hr]	-5.700e+007	-9.656e+007	-1.393e+008	-1.869e+008	-2.534
Name	RecyProds	Glycol	Reactor Prods	** New **	
Vapour Fraction	0.0000	0.0000	0.0000		
Temperature [F]	159.0	375.7	140.0		
Pressure [psia]	15.00	17.00	16.17		
Molar Flow [lbmole/hr]	475.8	142.8	618.5		
Mass Flow [lb/hr]	9890	1.082e+004	1.971e+004		
Liquid Volume Flow [USGPM]	17.97	20.78	38.75		
Heat Flow [Btu/hr]	-5.700e+007	-2.803e+007	-8.714e+007		

2. When you are finished in the column environment, return to the Main Flowsheet by clicking the **Enter Parent Simulation Environment** icon.

Enter Parent Simulation Environment Icon

3. Open the PFD for the Main Flowsheet and select **Auto Position All** from the **PFD** menu. HYSYS arranges your PFD in a logical manner.

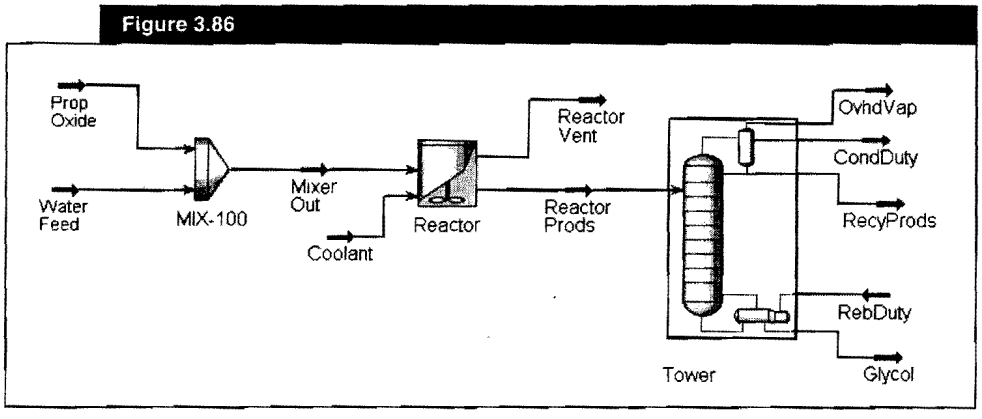
Moving Objects and Labels in a PFD

The PFD below has been customized by moving some of the stream icons. To move an icon, simply click and drag it to the new location.

You can also move a stream or operation label (name).

1. Right-click on the label you want to move.
2. From the menu that appears, select **Move/Size Label.** A box appears around the label.
3. Click and drag the label to a new location, or use the arrow keys to move it.

Figure 3.86

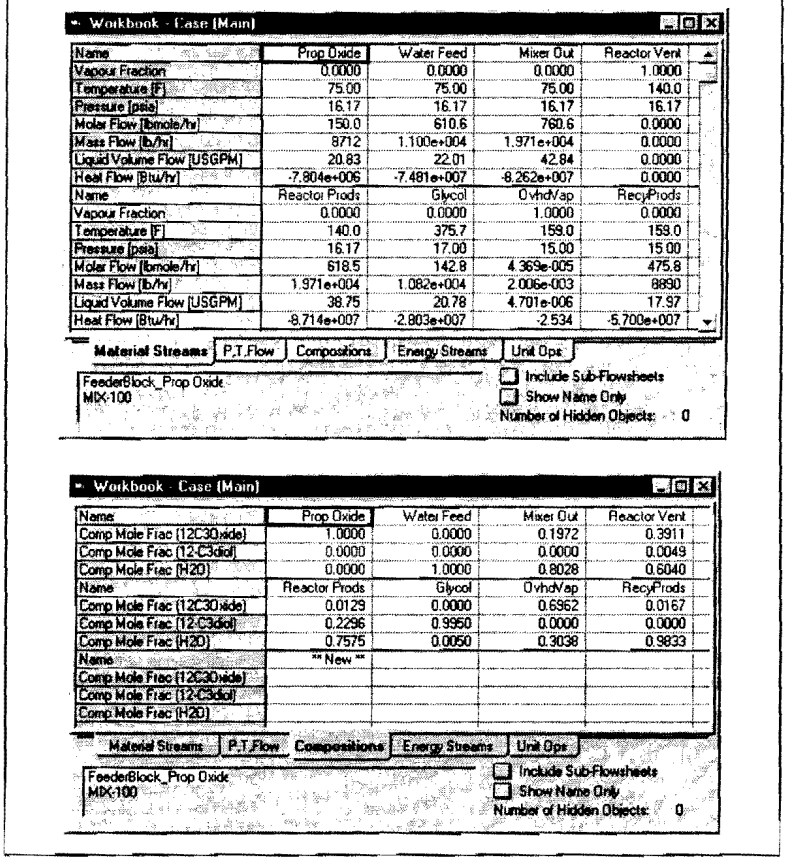


3.2.8 Viewing Results

1. Click the **Workbook** icon to access the calculated results for the Main Flowsheet.

The Material Streams tab and Compositions tab of the Workbook appears below.

Figure 3.87



Using the Object Navigator

If you want to view the calculated properties of a particular stream or operation, you can use the Object Navigator to quickly access the property view for any stream or unit operation at any time during the simulation.

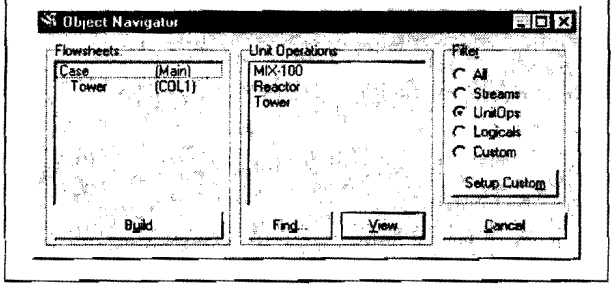
To open the Navigator, do **one** of the following:

- Press **F3**.
- From the Flowsheet menu, select **Find Object**.
- Double-click on any blank space on the HYSYS Desktop.
- Click the **Navigator** icon.

Navigator Icon

The Object Navigator view appears.

Figure 3.88



You can control which objects appear by selecting a different Filter radio button. For example, to list all streams and unit operations, select the **All** button.

The UnitOps radio button in the Filter group is currently selected, so only the Unit Operations appear in the list of objects.

To open a property view, select the operation in the list, then click the View button or double-click on the operation name.

You can start or end the search string with an asterisk (*), which acts as a wildcard character. This lets you find multiple objects with one search. For example, searching for VLV* will open the property view for all objects with VLV at the beginning of their name.

You can also search for an object by clicking the Find button.

When the Find Object view appears, enter the object name, then click the OK button.HYSYS opens the property view for the object you specified

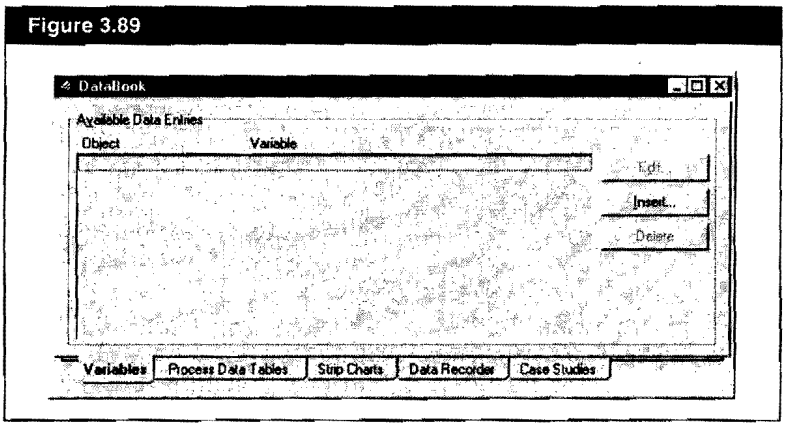
Using the Databook

The HYSYS Databook provides you with a convenient way to examine your flowsheet in more detail. You can use the Databook to monitor key variables under a variety of process scenarios, and view the results in a tabular or graphical format.

1. Before opening the Databook, close the Object Navigator and any property views you might have opened using the Navigator.
2. To open the Databook, do **one** of the following:
   - Press **CTRL D**.
   - From the **Tools** menu, select **Databook**.

The Databook view appears.

Figure 3.89



To edit any of the Objects in the Databook:

1. Select the Object you want to edit.
2. Click the **Edit** button.

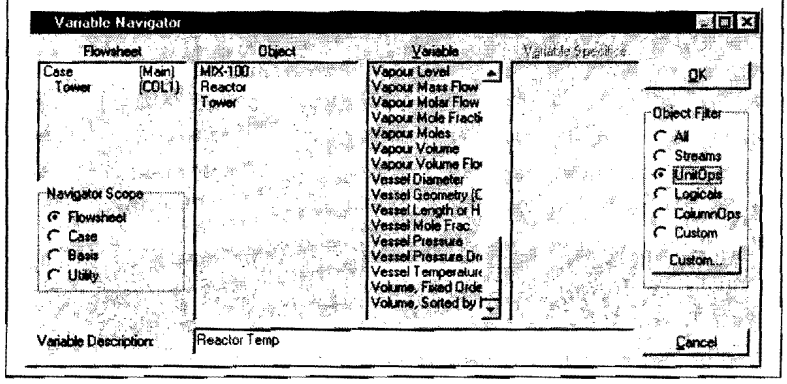
The first task is to add key variables to the Databook. For this example, the effects of the Reactor temperature on the Reactor cooling duty and Glycol production rate will be examined.

3. On the **Variables** tab, click the **Insert** button. The Variable Navigator appears.
4. In the Object Filter group, select the **UnitOps** radio button. The Object list is filtered to show unit operations only.
5. In the Object list, select Reactor. The variables available for the Reactor object appear in the Variable list.

The Variable Navigator is used extensively in HYSYS for locating and selecting variables. The Navigator operates in a left-to-right manner—the selected Flowsheet determines the Object list, the chosen Object dictates the Variable list, and the selected Variable determines whether any Variable Specifics are available.

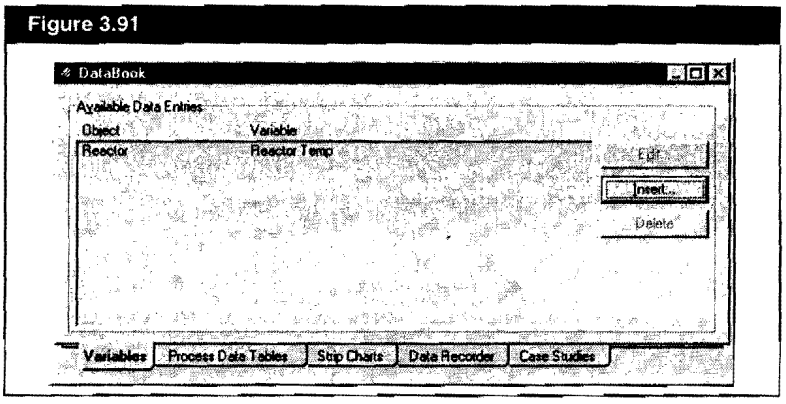
6. In the Variable list, select Vessel Temperature. Vessel Temperature appears in the **Variable Description** field. You can edit the default variable description.

Figure 3.90



7. In the **Variable Description** field, rename the variable Reactor Temp, then click the **OK** button. The variable now appears in the Databook.

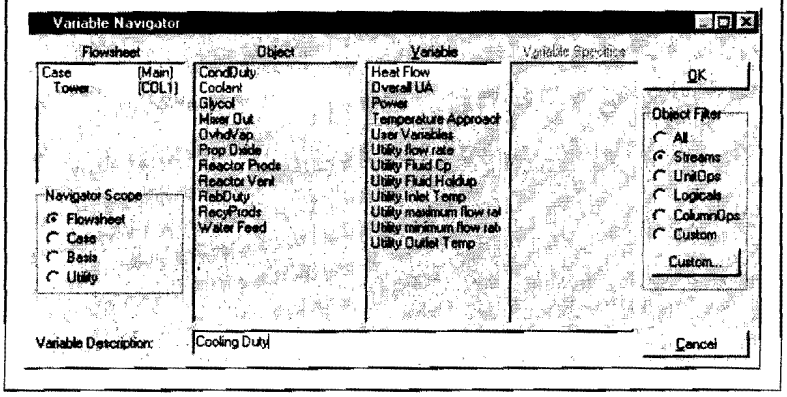
Figure 3.91



8. To add the next variable, click the **Insert** button. The Variable Navigator appears.
9. In the Object Filter group, select the **Streams** radio button. The Object list is filtered to show streams only.
10. In the Object list, select Coolant in the Object list. The variables available for this stream appear in the Variable list.

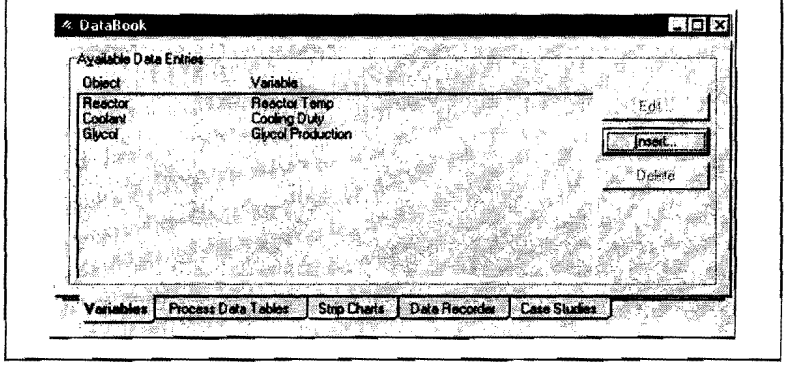
11. In the Variable list, select Heat Flow.

Figure 3.92



12. In the **Variable Description** field, change the description to Cooling Duty, then click the **OK** button. The variable now appears in the Databook.
13. Click the **Insert** button again. In the Object list, select Glycol. In the Variable list, select Liq Vol Flow@Std Cond. Change the **Variable Description** for this variable to Glycol Production, then click the **OK** button. The completed **Variables** tab of the Databook appears below.

Figure 3.93



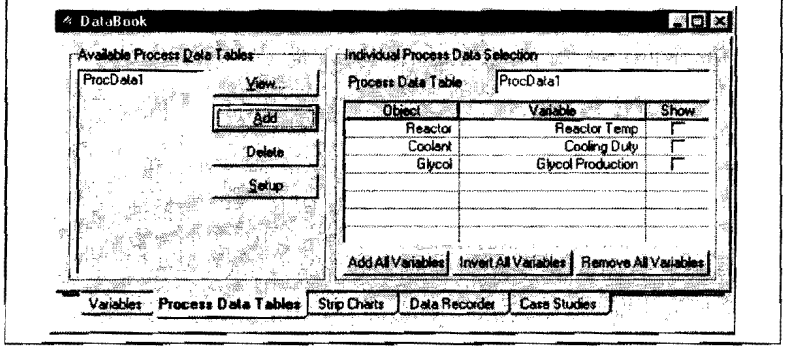
Now that the key variables have been added to the Databook, the next task is to create a data table in which to display these variables.

14. Click the **Process Data Tables** tab.

The three variables that you added to the Databook appear in the table on this tab.

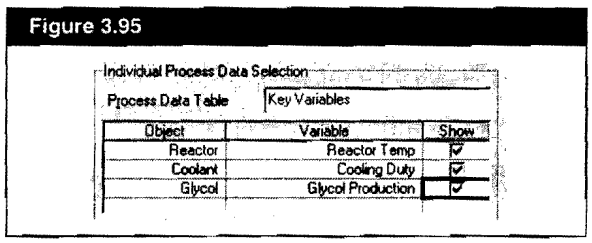
15. In the Available Process Data Tables group, click the **Add** button. HYSYS creates a new table with the default name ProcData1.

Figure 3.94



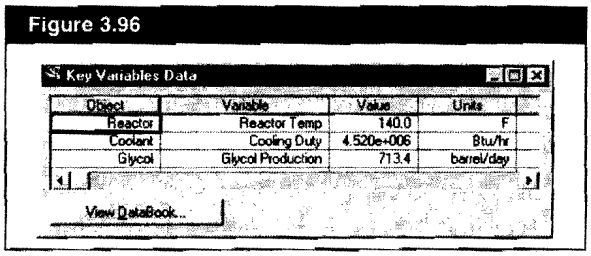
16. In the **Process Data Table** field, change the name to Key Variables.
17. In the Show column, activate each variable by clicking on the corresponding checkbox.

Figure 3.95



18. Click the **View** button to view the new data table.

Figure 3.96



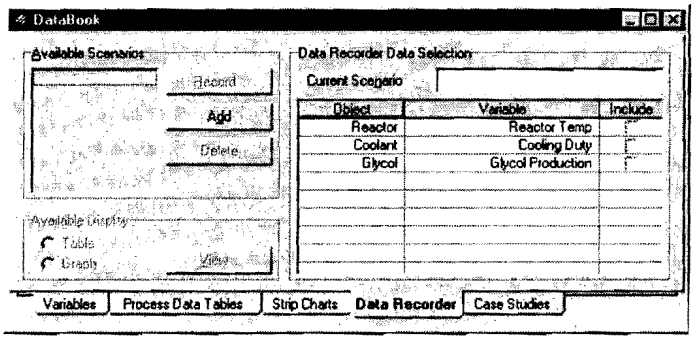
This table will be accessed again later to demonstrate how its results are updated whenever a flowsheet change is made.

19. For now, click the **Minimize** icon in the upper right corner of the Key Variables Data view. HYSYS reduces the view to an icon and places it at the bottom of the Desktop.

Before you make changes to the flowsheet, you will record the current values of the key variables. Instead of manually recording the variables, you can use the Data Recorder to automatically record them for you.

20. Click the Data **Recorder** tab in the Databook.

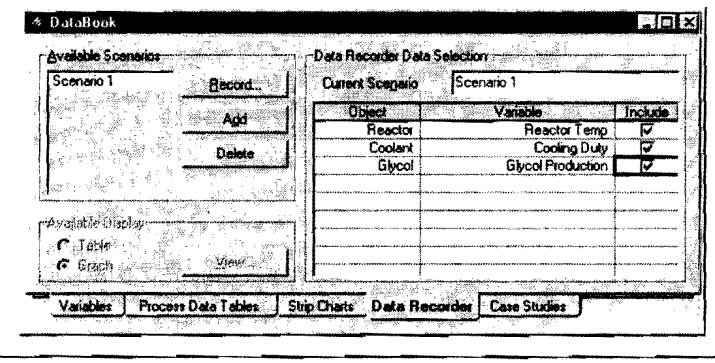
Figure 3.97

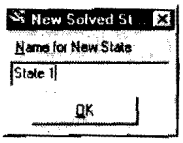


When using the Data Recorder, you first create a Scenario containing one or more of the key variables, then record the variables in their current state.

21. In the Available Scenarios group, click the **Add** button. HYSYS creates a new scenario with the default name Scenario 1.
22. In the Data Recorder Data Section group, activate each variable by clicking on the corresponding **Include** checkbox.

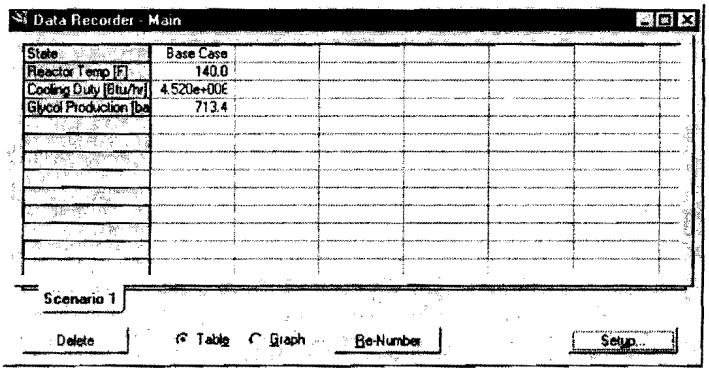
Figure 3.98





23. Click the **Record** button to record the variables in their current state. The New Solved State view appears, prompting you for the name of the new state.
24. In the **Name for New State** field, change the name to Base Case, then click **OK**. You return to the Databook.
25. In the Available Display group, select the **Table** radio button, then click the **View** button. The Data Recorder view appears, showing the values of the key variables in their current state.

Figure 3.99



Now you can make the necessary flowsheet changes and these current values remain as a permanent record in the Data Recorder unless you choose to erase them.

26. Click the **Minimize** icon on the Data Recorder view.
27. Click the **Restore Up** icon on the Key Variables Data title bar to restore the view to its regular size.

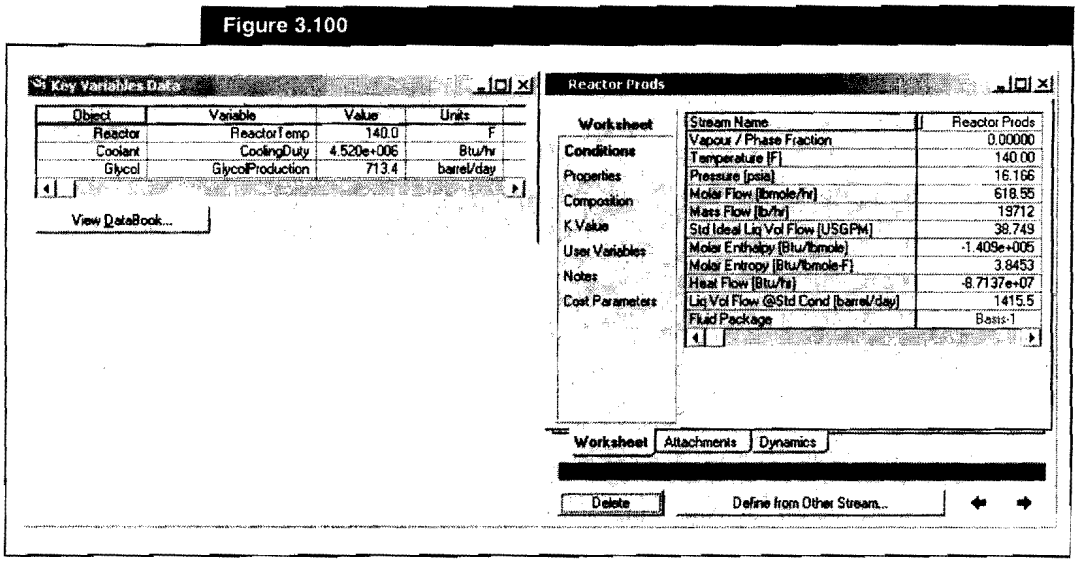
Next, you will change the temperature of stream Reactor Prods (which determines the Reactor temperature), then view the changes in the process data table

Navigator Icon

28. Click the **Navigator** icon in the toolbar.
29. In the Filter group, select the **Streams** radio button.
30. In the Streams list, select Reactor Prods, then click the **View** button. The Reactor Prods property view appears.
31. Ensure you are on the **Worksheet** tab, **Conditions** page of the property view.

32. Arrange the Reactor Prods and Key Variables Data views so you can see them both.

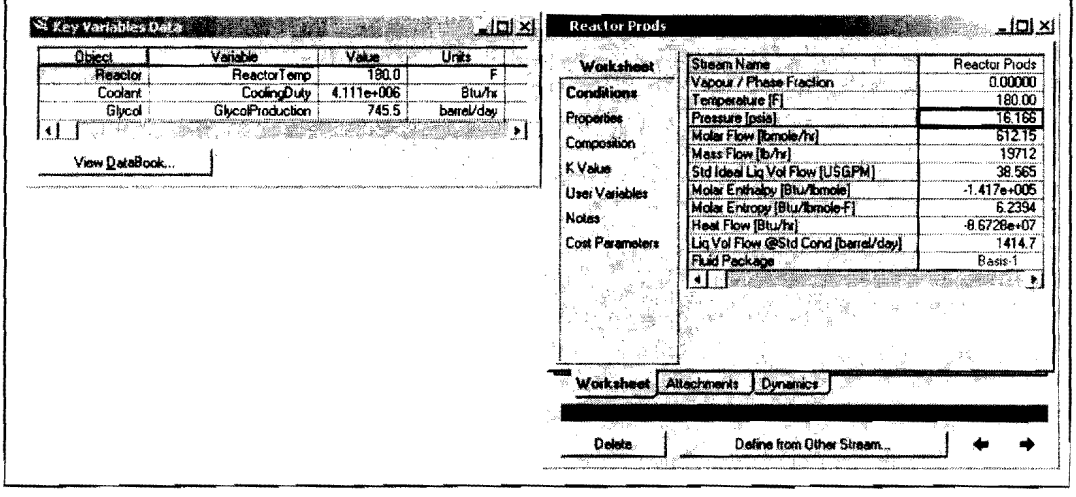
Figure 3.100



Currently, the Reactor temperature is 140°F. The key variables will be checked at 180°F.

33. In the Reactor Prods property view, change the value in the **Temperature** cell to 180. HYSYS automatically recalculates the flowsheet. The new results appears below.

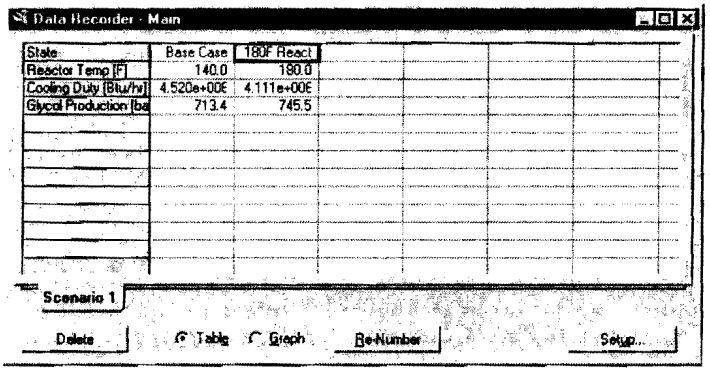
Figure 3.101



As a result of the change, the required cooling duty decreased and the glycol production rate increased.

34. Click the **Close** button on the Reactor Prods stream property view to return to the Databook. You can now record the key variables in their new state.
35. Click on the **Data Recorder** tab in the Databook.
36. Click the **Record** button. The New Solved State view appears.
37. In the **Name for New State** field, change the name to 180F Reactor, then click the **OK** button.
38. In the Available Display group, click the **View** button. The Data Recorder appears, displaying the new values of the variables.

Figure 3.102



39. Close the Data Recorder view, then the Databook view, and finally the Key Variables Data view.

This completes the HYSYS Chemicals Steady State Simulation tutorial. If there are any aspects of this case that you would like to explore further, feel free to continue working on this simulation on your own.

Further Study

For other chemical case examples, see the Applications section. Applications beginning with "C" explore some of the types of chemical simulations that can be built using HYSYS.

5.2.5 Reactions Tab

See **Chapter 5 - Reactions** in the Simulation Basis manual for more information.

The Reactions Tab in the Simulation Basis Manager allows you to define reactions within HYSYS. You can define an unlimited number of reactions and group these reactions in reaction sets. The reaction sets are then attached to unit operations in the flowsheet.

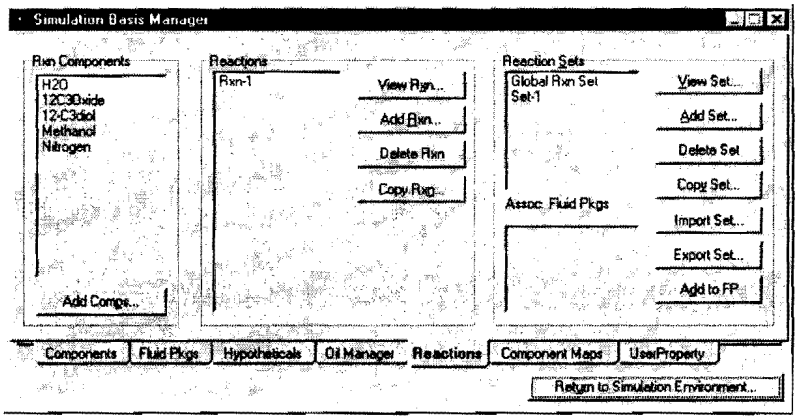
Any ReactionSet and Reaction in the Reaction Manager bank cannot be attached to any unit operation in an electrolyte flowsheet (reactor unit operations are disabled).

The electrolytes thermo calculation conducts a reactive and phase flash at the same time. Therefore, adding any external reactions to a unit operation is not yet allowed in HYSYS for electrolyte simulation.

For more information, refer to the HYSYS Electrolytes OLI manual.

The Reaction tab appears as shown in the following figure.

Figure 5.8



Use the Reaction Manager to do the following:

- Create a new list of components for the reactions or use the components associated with a fluid package.
- Add, Edit, Copy or Delete reactions and reaction sets.
- Attach reactions to various reaction sets, or attach reaction sets to multiple fluid packages.
- Import and Export reaction sets.

Adding a Reaction

1. Click the **Add Rxn** button. The Reactions view appears.
2. Select the type of reaction that you want to use.
3. Click the **Add Reaction** button. The Reaction Property view appears; in this view, you can define the following:
   - Stoichiometry
   - Conversion basis
   - Equilibrium constant
   - Other properties
4. Click the **Stoichiometry** tab.
5. Click the field that displays **Add Comp**. Select the component you want to use for the reaction from the drop-down list.
6. Repeat the previous step until all of the required components are added to the table.
7. In the Stoich Coeff column, enter a stoichiometric coefficient for each component. This value must be negative for a reactant and positive for a product.
8. Specify the coefficient for an inert component as 0 (which for the Conversion reaction is the same as not including the component in the table). Fractional coefficients are acceptable.

Editing a Reaction

1. From the list of available reactions, select the reaction you want to edit.
2. Click the **View Rxn** button. The Reaction Property view appears. In this view, you can modify the following:
   - Stoichiometry
   - Conversion basis
   - Equilibrium constant
   - Other properties

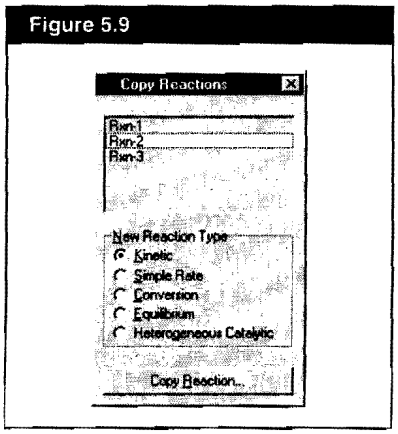
Deleting a Reaction

1. From the list of available reactions, select the reaction you want to delete.
2. Click the **Delete Rxn** button. HYSYS prompts you to confirm the deletion.

Copying a Reaction

1. From the list of available reactions, select the reaction you want to copy.
2. Click the **Copy Rxn** button. The Copy Reactions view appears.

Figure 5.9



3. Select the reaction you want to copy from the list of reactions.
4. Use the radio buttons in the New Reaction Type group to select the reaction type for the reaction copy.
5. Click the **Copy Reaction** button.

Adding a Reaction Set

1. Click the **Add Set** button. The Reaction Set view appears.
2. In the Active List column, click the <empty> cell and use the drop-down list to select the reaction you want to add to the set.
3. In the Inactive List column, click the <empty> cell and use the drop-down list to select the reaction you want to add to the set. This reaction remains inactive, but it is included in the set.
4. From the Solver Method drop-down list, select the reaction solver method you want to use.

Available reaction solver methods:

- Newton's Method
- Rate Iterated
- Rate Integrated
- Auto Select

5. Add any of the available reactions to the set (as long as they are the same type). A single reaction can be added to as many sets as necessary.

Editing a Reaction Set

1. From the list of available reaction sets, select the reaction set you want to edit.
2. Click the **View Set** button. The Reaction Set view appears. In this view, you can do the following:
   - Add and remove reactions in the reaction set.
   - Modify the solver method.
   - Activate and inactivate reactions already in the set.

Deleting a Reaction Set

1. From the list of available reaction sets, select the reaction set you want to delete.
2. Click the **Delete** button. HYSYS prompts you to confirm the deletion of the reaction set.

Copying a Reaction Set

1. From the list of available reaction sets, select the reaction set you want to copy.
2. Click the **Copy** button.

Copying a reaction set creates a new reaction set with the exact same properties as the original.

Importing a Reaction Set

1. Click the **Import Set** button. The Open File view appears.
2. Browse to the location of your reaction sets file (*.rst).
3. Select the file you want to import, then click **Open**.

Exporting a Reaction Set

1. Click the **Export Set** button. The Save File view appears.
2. Specify the name and location of your reaction set file.
3. Click **Save**.

Adding a Reaction Set to a Fluid Package

After creating reactions and reaction sets, you can associate the set(s) with a fluid package.

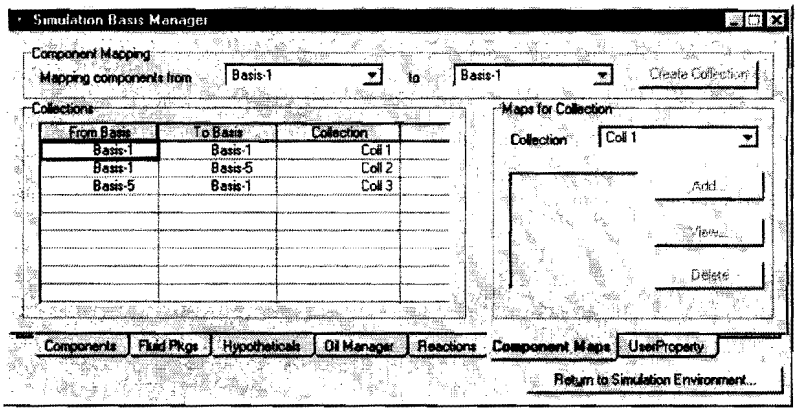
1. Click the **Add to FP** button. The Add Reaction Set view appears.
2. From the list of available fluid packages, select the fluid package to which you want to add a reaction set.
3. Click the **Add Set to Fluid Package** button.

5.2.6 Component Maps Tab

See **Chapter 6 - Component Maps** in the Simulation Basis manual for additional information.

The Component Maps tab allows you to map fluid component composition across fluid package boundaries. Composition values for individual components from one fluid package can be mapped to a different component in an alternate fluid package. This is useful when dealing with hypothetical oil components.

Figure 5.10



Two previously defined fluid packages are required to perform a component mapping. One fluid package becomes the target component set and the other becomes the source component set. Mapping is performed using a matrix of source and target components. The transfer basis can be performed on a mole, mass or liquid volume basis.

5.3 Reactions

Refer to **Section 5.4 - Reaction Sets** for information on Reaction Sets.

In HYSYS, a default reaction set, the Global Rxn Set, is present in every simulation. All compatible reactions that are added to the case are automatically included in this set. A Reaction can be attached to a different set, but it also remains in the Global Rxn Set unless you remove it. To create a Reaction, click the Add Rxn button from the Reaction Manager.

The following table describes the five types of Reactions that can be modeled in HYSYS:

Reaction Type	Requirements
Conversion	Requires the stoichiometry of all the reactions and the conversion of a base component in the reaction.
Equilibrium	Requires the stoichiometry of all the reactions. The term Ln(K) may be calculated using one of several different methods, as explained later. The reaction order for each component is determined from the stoichiometric coefficients.
Heterogeneous Catalytic	Requires the kinetics terms of the Kinetic reaction as well as the Activation Energy, Frequency Factor and Component Exponent terms of the Adsorption kinetics.
Kinetic	Requires the stoichiometry of all the reactions, as well as the Activation Energy and Frequency Factor in the Arrhenius equation for forward and reverse (optional) reactions. The forward and reverse orders of reaction for each component can be specified.
Simple Rate	Requires the stoichiometry of all the reactions, as well as the Activation Energy and Frequency Factor in the Arrhenius equation for the forward reaction. The Equilibrium Expression constants are required for the reverse reaction.

Each of the reaction types require that you supply the stoichiometry. To assist with this task, the Balance Error tracks the molecular weight and supplied stoichiometry. If the reaction equation is balanced, this error is equal to zero. If you have provided all of the stoichiometric coefficients except one, you may select the Balance button to have HYSYS determine the missing stoichiometric coefficient.

Reactions can be on a phase specific basis. The Reaction is applied only to the components present in that phase. This allows different rate equations for the vapour and liquid phase in same reactor operation.

5.3.1 Manipulating Reactions

When you object inspect a reaction in the Reactions group, you can select View or Delete from the menu.

From the Reaction Manager, you can use the four buttons in the Reactions group to manipulate reactions. The buttons are described below:

Button	Command
View Rxn	Accesses the property view of the highlighted reaction.
Add Rxn	Accesses the **Reactions** view, from which you select a Reaction type.
Delete Rxn	Removes the highlighted reaction(s) from the Reaction Manager.
Copy Rxn	When selected, the Copy Reactions view appears where you can select an alternate Reaction Type for the reaction or duplicate the highlighted reaction.

5.3.2 Conversion Reaction

By default, conversion reactions are calculated simultaneously. However you can specify sequential reactions using the Ranking feature. See **Section 5.4 - Reaction Sets**.

The Conversion Reaction requires the Stoichiometric Coefficients for each component and the specified Conversion of a base reactant. The compositions of unknown streams can be calculated when the Conversion is known.

Consider the following Conversion reaction:

$$A + \frac{b}{a}B \rightarrow \frac{c}{a}C + \frac{d}{a}D \qquad (5.1)$$

where: a, b, c and d are the respective stoichiometric coefficients of the reactants (A and B) and products (C and D).

A is the base reactant and B is not in a limiting quantity.

In general, the reaction components obey the following reaction stoichiometry:

$$
\begin{aligned}
N_A &= N_{A_o}(1 - X_A) \\
N_B &= N_{B_o} - \frac{b}{a} N_{A_o} X_A \\
N_C &= N_{C_o} + \frac{c}{a}(N_{A_o} X_A) \\
N_D &= N_{D_o} + \frac{d}{a}(N_{A_o} X_A)
\end{aligned}
\qquad (5.2)
$$

where: $N_* =$ *The final moles of component * (*= A, B, C and D)*

$N_{*_o} =$ *The initial moles of component **

$X_A =$ *The conversion of the base component A*

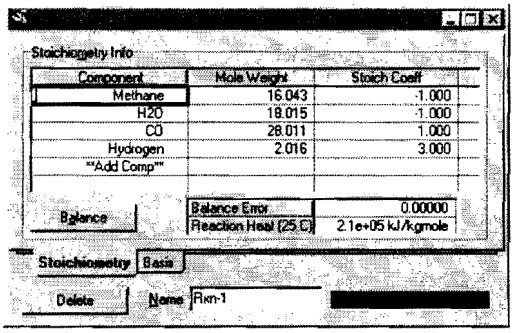
When you have supplied all of the required information for the Conversion Reaction, the status message will change from Not Ready to Ready.

The moles of a reactant available for conversion in a given reaction include any amount produced by other reactions, as well as the amount of that component in the inlet stream(s). An exception to this occurs when the reactions are specified as sequential.

Stoichiometry Tab

The Stoichiometry tab of a conversion reaction is shown in the figure below:

Figure 5.3



For each Conversion reaction, you must supply the following information:

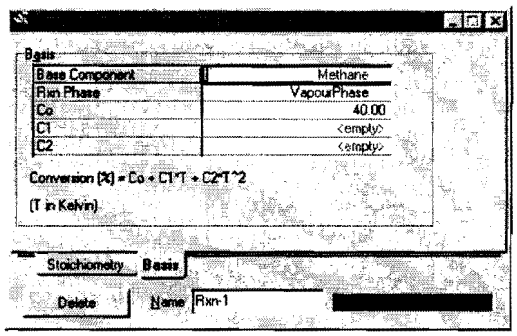
Input Field	Information Required
Reaction Name	A default name is provided which may be changed. The previous view shows the name as Rxn-1.
Components	The components to be reacted. A minimum of two components are required. You must specify a minimum of one reactant and one product for each reaction you include. Use the drop-down list to access the available components. The Molecular Weight of each component is automatically displayed.
Stoichiometric Coefficient	Necessary for every component in the reaction. The Stoichiometric Coefficient is negative for a reactant and positive for a product. You may specify the coefficient for an inert component as 0, which, for the Conversion reaction, is the same as not including the component in the table. The Stoichiometric Coefficient does not have to be an integer; fractional coefficients are acceptable.

The Reaction Heat value is calculated and displayed below the Balance Error. A positive value indicates that the reaction is endothermic.

Basis Tab

The Basis tab of a conversion reaction is shown in the figure below:

Figure 5.4



On the Basis tab, you must supply the following information:

Required Input	Description
Base Component	Only a component that is consumed in the reaction (a reactant) may be specified as the Base Component (i.e., a reaction product or an inert component is not a valid choice). You can use the same component as the Base Component for a number of reactions, and it is quite acceptable for the Base Component of one reaction to be a product of another reaction. Note that you have to add the Components to the reaction before the Base Component can be specified.
Rxn Phase	The phase for which the specified conversions apply. Different kinetics for different phases can be modeled in the same reactor. Possible choices for the Reaction Phase are: • **Overall**. Reaction occurs in all Phases. • **Vapour Phase**. Reaction occurs only in the Vapour Phase. • **Liquid Phase**. Reaction occurs only in the Light Liquid Phase. • **Aqueous Phase**. Reaction occurs only in the Heavy Liquid Phase. • **Combined Liquid**. Reaction occurs in all Liquid Phases.
Conversion Function Parameters	Conversion percentage can be defined as a function of reaction temperature according to the following equation: $Conv = Co + C1 \cdot T + C2 \cdot T^2$ This is the percentage of the Base Component consumed in this reaction. The value of *Conv.(%)* calculated from the equation is always limited within the range of 0.0 and 100%. The actual conversion of any reaction is limited to the lesser of the specified conversion of the base component or complete consumption of a limiting reactant.

Sequential Reactions may be modeled in one reactor by specifying the sequential order of solution. See Reaction Rank, in **Section 5.4 - Reaction Sets**.

Note that reactions of equal ranking cannot exceed an overall conversion of 100%.

To define a constant value for conversion percentage, enter a conversion (%) value for *Co* only. Negative values for *C1* and *C2* means that the conversion drops with increased temperature and vice versa.

Conversion Reactor icon

9.2.2 Conversion Reactor Reactions Tab

The Conversion Reactor is a vessel in which conversion reactions are performed. You can only attach reaction sets that contain conversion reactions. Each reaction in the set proceeds until the specified conversion is attained or until a limiting reactant is depleted.

Refer to **Section 5.3.2 - Conversion Reaction** in the **Simulation Basis** manual for details on creating Conversion Reaction Sets and Conversion Reactions.

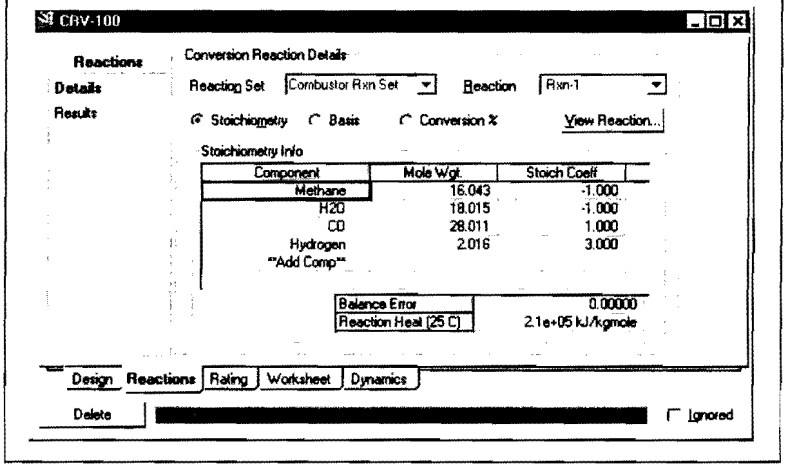
The Reactions tab, consists of two pages:

- Details
- Results.

Details Page

You can attach the reaction set to the operation and specify the conversion for each reaction in the set on the Details page. The reaction set can contain only conversion reactions.

Figure 9.5



The Details page consists of four objects as described in the table below.

Object	Description
Reaction Set	Allows you to select the appropriate conversion reaction set.
Reaction	You must select the appropriate conversion reaction from the selected Reaction Set.

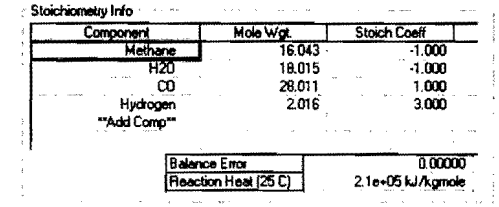
Object	Description
View Reaction button	Opens the Reaction property view for the reaction currently selected in the Reaction drop-down list. The Reaction property view allows you to edit the reaction.
[Radio buttons]	The three radio buttons on the Details page are: • Stoichiometry • Basis • Conversion The three radio buttons allow you to toggle between the Stoichiometry group, the Basis group or the Conversion group (each group is described in the following sections).

Stoichiometry Radio Button

The Balance Error (for the reaction stoichiometry) and the Reaction Heat (Heat of Reaction at 25°C) are also shown for the current reaction.

When you select the Stoichiometry radio button, the Stoichiometry Info group appears. The Stoichiometry Info group allows you to examine the components involved in the selected reaction, their molecular weights as well as their stoichiometric coefficients.

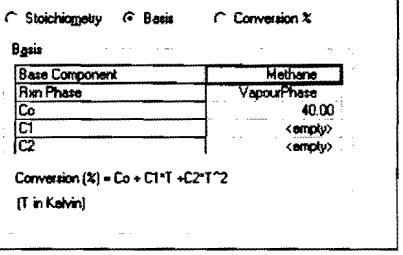
Figure 9.6



Basis Radio Button

When you select the Basis radio button, the Basis group appears. In the Basis group, you can view the base component, the conversion, and the reaction phase for each reaction in the reaction set.

Figure 9.7

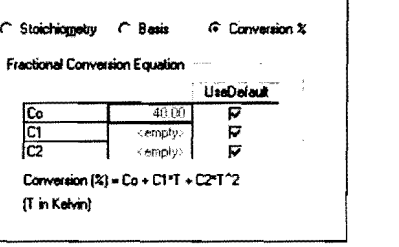


Conversion Radio Button

In the Fractional Conversion Equation group, parameters shown in red or blue colour indicate that the variable can be cloned.

When you select the Conversion radio button, the Fractional Conversion Equation group appears. The Fractional Conversion Equation group allows you to implement a conversion model based on the *Conversion(%)* equation listed.

Figure 9.8

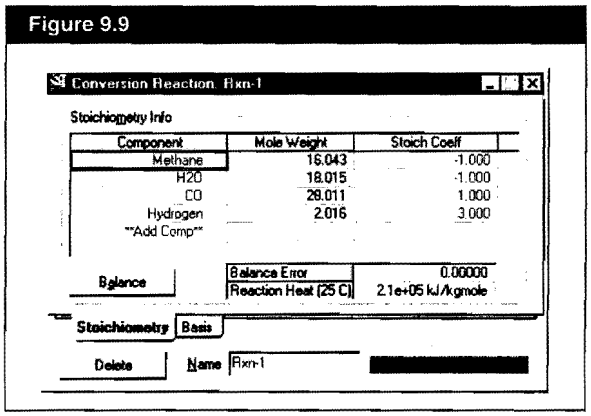


The parameters for the attached conversion reaction(s) can be cloned as local variables belonging to the Conversion Reactor. Therefore, you can either use the parameters specified in the reaction(s) from the attached reaction set by clicking the Use Default checkbox or specifying locally the values within the Fractional Conversion Equation group.

View Reaction Button

When you click the View Reaction button, the Conversion Reaction property view of the reaction currently selected in the Reaction drop-down list appears.

Figure 9.9



Any changes made to the Conversion Reaction property view are made globally to the selected Reaction and any Reaction Sets which contain the Reaction. For example, if any change is made to the reaction shown in the figure above, the change is carried over to every other instance in which this Reaction is used. It is therefore recommended that changes which are Reactor specific (i.e., changes which are only meant to affect one Reactor) are made within the Reactions tab.

Results Page

You can change the specified conversion for a reaction directly on this page.

The Results page displays the results of a converged reactor. The page consists of the Reactor Results Summary group which contains two radio buttons:

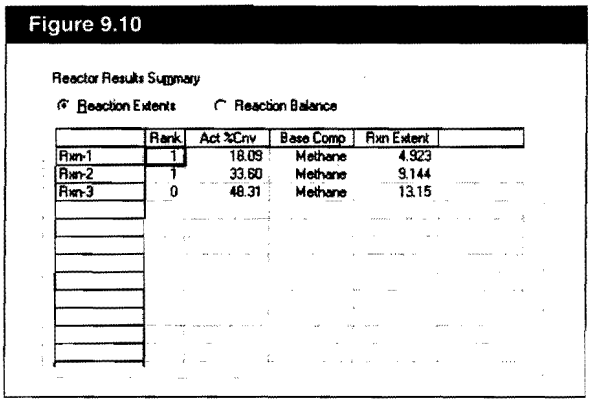
- Reaction Extents
- Reaction Balance.

The type of results displayed on the Results page depend on the radio button selected.

Reaction Extents Radio Button

When the Reaction Extents radio button is selected, the Results page appears as shown in the figure below.

Figure 9.10



The Reactor Results Summary group displays the following results for a converged reactor:

When there are multiple reactions in a Reaction Set, HYSYS automatically ranks the reactions. A reaction with a lower ranking value occurs first. Each group of reactions of *equal rank* can have an overall specified conversion between 0% and 100%.

Result Field	Description
Rank	Displays the current rank of the reaction. For multiple reactions, lower ranked reactions occur first.
Actual % Conversion	Displays the percentage of the base component in the feed stream(s) which has been consumed in the reaction.
Base Component	The reactant to which the calculation conversion is based on.
Rxn Extent	Lists the molar rate consumption of the base component.

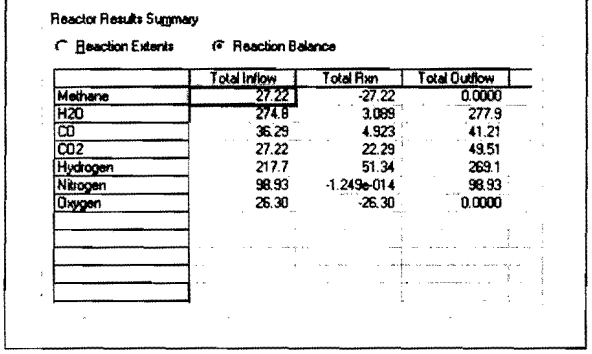
Any changes made to the global reaction affect all Reaction Sets to which the reaction is attached, provided local changes have not been made.

Notice that the actual conversion values do not match the specified conversion values. Rxn-3 proceeds first and is halted when a limiting reactant is exhausted. The sum of the specified conversions for Rxn-1 and Rxn-2 is 100%, so all of the remaining base component can be consumed, provided a limiting reactant is not fully consumed beforehand. All of the base component is consumed, and this is reflected in the actual conversion totalling 100%.

Reaction Balance Radio Button

When the Reaction Balance radio button is selected, the Reaction Balance option provides an overall component summary for the Conversion Reactor. All components which appear in the fluid package are shown here.

Figure 9.11



	Total Inflow	Total Rxn	Total Outflow
Methane	27.22	-27.22	0.0000
H2O	274.8	3.089	277.9
CO	36.29	4.923	41.21
CO2	27.22	22.29	49.51
Hydrogen	217.7	51.34	269.1
Nitrogen	98.93	-1.249e-014	98.93
Oxygen	26.30	-26.30	0.0000

Values appear after the solution of the reactor has converged. The Total Inflow rate, the Total Reacted rate and the Total Outflow rate for each component are provided on a molar basis. Negative values indicate the consumption of a reactant, while positive values indicate the appearance of a product.

9.2.3 CSTR Reactions Tab

For more information on Kinetic, Heterogeneous Catalytic and Simple Rate reactions, refer to **Chapter 5 - Reactions** in the **Simulation Basis** manual.

CSTR icon

The CSTR is a vessel in which Kinetic, Heterogeneous Catalytic, and Simple Rate reactions can be performed. The conversion in the reactor depends on the rate expression of the reactions associated with the reaction type. The inlet stream is assumed to be perfectly (and instantaneously) mixed with the material already in the reactor, so that the outlet stream composition is identical to that of the reactor contents. Given the *reactor volume*, a *consistent rate expression* for each reaction and the *reaction stoichiometry*, the CSTR computes the conversion of each component entering the reactor.