UniSim® Design

Tutorials and Applications

Honeywell

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A UniSim Design Tutorials

The Tutorials section of this guide presents you with independent tutorial sessions. Each tutorial guides you step-by-step through the complete construction of a UniSim Design simulation. The tutorial(s) you choose to work through will likely depend on the simulation topic that is most closely related to your work, your familiarity with UniSim Design, and the types of simulation cases you anticipate on creating in the future.

All completed Tutorial cases are included with your UniSim Design package, and are available on UniSim Design\Samples folder.

Regardless of which tutorial you work through first, you will gain the same basic understanding of the steps and tools used to build a UniSim Design simulation. After building one of these tutorial cases, you might choose to build one or several more, or begin creating your own simulations.

If you are new to UniSim Design, it is recommended that you begin with the steady state tutorials. These tutorials explicitly detail each step required to complete the simulation. In steps where more than one method is available to complete a particular action, all methods are outlined. The dynamic tutorials (which are continued after the steady state section) are also presented in a step-by-step manner, but are less detailed in their explanations. They assume a rudimentary knowledge of the UniSim Design interface and methods.

The three tutorials are grouped in three general areas of interest:

- Gas Processing
- Refining
- Chemicals

Each area has an associated steady state and dynamic tutorial. The dynamic tutorials use the steady state cases and add control schemes and dynamic specifications required to run the case in Dynamic mode. If you are interested only in steady state simulation, go through the steady state tutorial(s) that most interest you and stop at the dynamics section. If you are interested only in learning to apply dynamic simulation methods, use the pre-built steady state base case, included with UniSim Design, as the starting point for your dynamic tutorial

case.

Introduction

There are also several UniSim Design training courses available. Contact Honeywell for more information, or visit our web site **www.honeywell.com**.

In the chapters that follow, example problems are used to illustrate some of the basic concepts of building a simulation in UniSim Design. Three complete tutorials are presented:

1. Gas Processing
   - **Steady State**. Models a sweet gas refrigeration plant consisting of an inlet separator, gas/gas heat exchanger, chiller, low-temperature separator and de-propanizer column.
   - **Dynamics**. Models the Gas Processing tutorial case in Dynamic mode. This tutorial makes use of the recommendations of the Dynamic Assistant when building the case.
2. Refining
   - **Steady State**. Models a crude oil processing facility consisting of a pre-flash drum, crude furnace and an atmospheric crude column.
   - **Dynamics**. Models the Refining example problem in Dynamic mode.
3. Chemicals
   - **Steady State**. Models a propylene glycol production process consisting of a continuously-stirred-tank reactor and a distillation tower.
   - **Dynamics**. Models the Chemicals example problem in Dynamic mode. This tutorial make use of the recommendations of the Dynamic Assistant when building the case.

The solved steady state cases are saved in the UniSim Design\Samples folder as TUTOR1.usc, TUTOR2.usc, and TUTOR3.usc files.

For the dynamics tutorials, you can use the pre-built steady state cases as your starting point. The solved dynamics cases are also included as dyntut1.usc, dyntut2.usc, and dyntut3.usc.

Each example contains detailed instructions for choosing a property package and components, installing and defining streams, unit operations and columns, and using various aspects of the UniSim Design interface to examine the results while you are creating the simulation.

Often in UniSim Design, more than one method exists for performing a task or executing a command. Many times you can use the keyboard, the mouse, or a combination of both to achieve the same result. The steady state tutorials attempt to illustrate UniSim Design's flexibility by showing you as many of these alternative methods as possible. You can then choose which approach is most appropriate for you.

The dynamics tutorials use the steady state solution as a basis for building the dynamic case. If you like, you can build the steady state case and then proceed with the dynamic solution, or you can simply call up the steady state case from disk and begin the dynamic modeling.

Starting UniSim Design

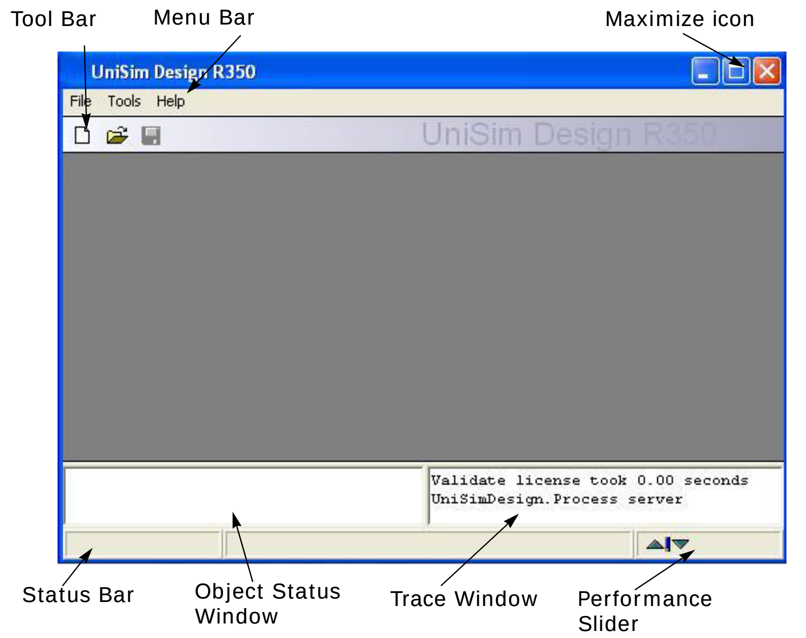
The installation process creates the following shortcut to UniSim Design:

1. Click on the **Start** menu.
2. Select **Programs | Honeywell | UniSim Design | UniSim Design R350**.

   The UniSim Design Desktop appears:

To learn more about the basics of the UniSim Design interface, refer to **Chapter 1 - Interface** in the **UniSim Design User Guide**.

Figure A.1



Getting Started

The tutorials start in Steady State mode, and end in Dynamic mode.

You are now ready to begin building a UniSim Design simulation, so

proceed to the Tutorial of your choice.

Tutorial	Chapter	Samples Case Name (Steady State / Dynamic)
Gas Processing	Chapter 1	TUTOR1.usc dyntut1.usc
Refining	Chapter 2	TUTOR2.usc dyntut2.usc
Chemicals	Chapter 3	TUTOR3.usc dyntut3.usc

Once you have completed one or more tutorials, you may want to examine the Applications section for other examples that may be of interest.

1 Gas Processing Tutorial

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1.1 Introduction

The gas processing simulation will be built using the following basic steps:

1. Create a unit set.
2. Choose a property package.
3. Select the components.
4. Create and specify the feed streams.
5. Install and define the unit operations prior to the column.
6. Install and define the column.

A solved case is located in the file **TUTOR1.usc** in your **UniSim Design\Samples** directory.

In this Tutorial, a natural gas stream containing **N2**, **CO2**, and **C1 through n-C4** is processed in a refrigeration system to remove the heavier hydrocarbons. The lean, dry gas produced will meet a pipeline hydrocarbon dew point specification. The liquids removed from the rich gas are processed in a depropanizer column, yielding a liquid product with a specified propane content.

The following pages will guide you through building a UniSim Design case to illustrate the complete construction of the simulation, from selecting a property package and components to examining the final results. The tools available in the UniSim Design interface will be utilized to illustrate the flexibility available to you.

Before proceeding, you should have read the introductory chapter which precedes the Tutorials in this guide.

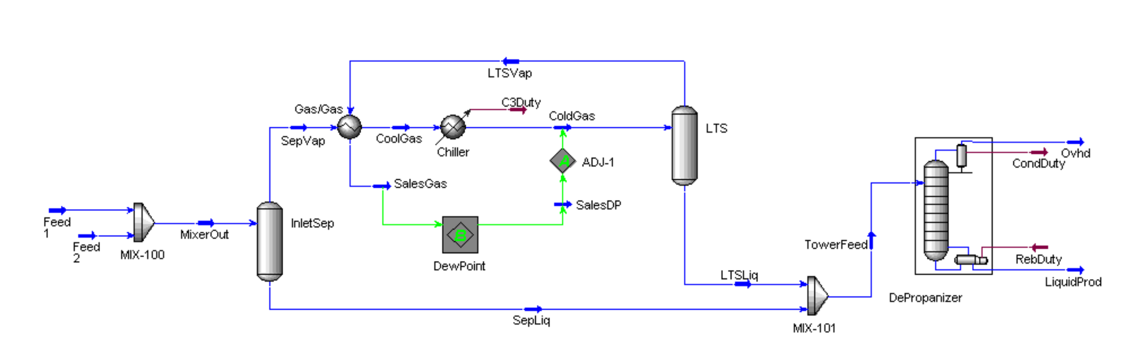
1.2 Steady State Simulation

1.2.1 Process Description

This tutorial will model a natural gas processing facility that uses propane refrigeration to condense liquids from the feed and a distillation tower to process the liquids. The flowsheet for this process

appears below.

Figure 1.1



The combined feed stream enters an inlet separator, which removes the free liquids. Overhead gas from the **Separator** is fed to the gas/gas exchanger, where it is pre-cooled by already refrigerated gas. The cooled gas is then fed to the chiller, where further cooling is accomplished through exchange with evaporating propane (represented by the **C3Duty** stream). In the chiller, which will be modeled simply as a **Cooler**, enough heavier hydrocarbons condense such that the eventual sales gas meets a pipeline dew point specification. The cold stream is then separated in a low-temperature separator (LTS). The dry, cold gas is fed to the gas/gas exchanger and then to sales, while the condensed liquids are mixed with free liquids from the inlet separator. These liquids are processed in a depropanizer column to produce a low-propane-content bottoms product.

Once the results for the simulation have been obtained, you will have a good understanding of the basic tools used to build a UniSim Design simulation case. At that point, you can either proceed with the Optional Study presented at the end of the tutorial or begin building your own simulations.

In this tutorial, three logical operations will be installed in order to perform certain functions that cannot be handled by standard physical unit operations:

Logical	Flowsheet Function
Balance	To duplicate the composition of the SalesGas stream in order to calculate its dew point temperature at pipeline specification pressure.
Adjust	To determine the required LTS temperature which gives a specified SalesGas dew point.
UniSim Design Spreadsheet	To calculate the SalesGas net heating value.

The **Balance** operation will be installed in the main example. In the

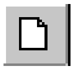
Optional Study section, the Adjust and Spreadsheet operations will be installed to investigate the effect of the LTS temperature on the sales gas heating value.

The two primary building tools, the **Workbook** and the **PFD**, will be 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 lot of flexibility in building your simulation and in quickly accessing the information you need.

The Workbook will be used to build the first part of the flowsheet, starting with the feed streams and building up to and including the gas/gas heat exchanger. The PFD will be used to install the remaining operations, from the chiller through to the column.

1.2.2 Setting Your Session Preferences

All commands on the toolbar are also available as menu items.

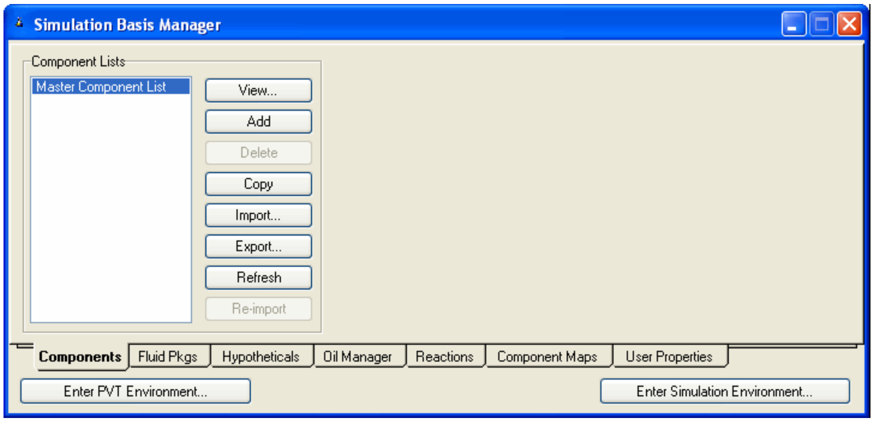


New Case icon

1. To start a new simulation case, do **one** of the following:
   - From the **File** menu, select **New** and then **Case**.
   - Click the **New Case** icon.

   The **Simulation Basis Manager** appears:

Figure 1.2

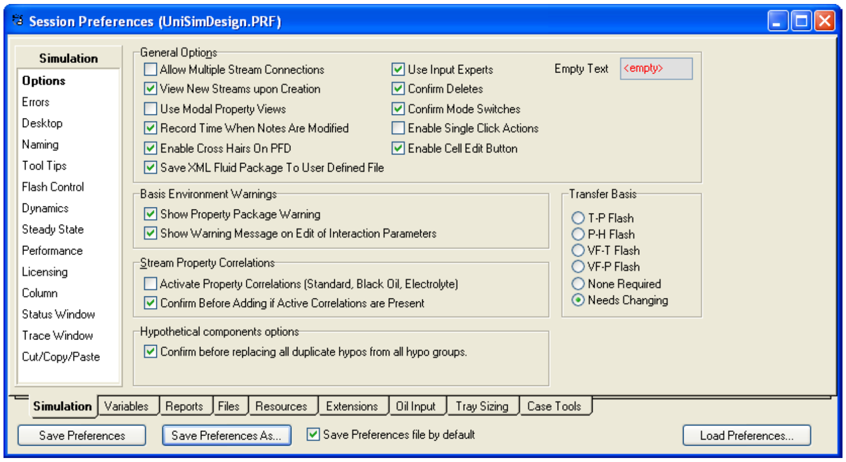


The Simulation Basis Manager view allows you to create, modify, and manipulate fluid packages in your simulation case. Most of the time, as with this example, you will require only one fluid package for your entire simulation.

Next, you will set your Session Preferences before building a case.

2. From the **Tools** menu, select **Preferences**. The Session Preferences view appears.You should be on the **Options** page of the **Simulation** tab.

Figure 1.3



The UniSim Design default session settings are stored in a Preference file called **unisimdesign R*.prf**. When you modify any of the preferences, you can save the changes in a new Preference file by clicking either **Save Preferences** which will overwrite the default file or **Save Preferences As...** and UniSim Design will prompt you to provide a name for the new Preference file. Click the **Load Preferences** button to load into any simulation case.

Check the **Save Preferences File by default** to automatically save the preference file when exiting UniSim Design.

3. In the General Options group, ensure the **Use Modal Property Views** checkbox is unchecked.

Creating a New Unit Set

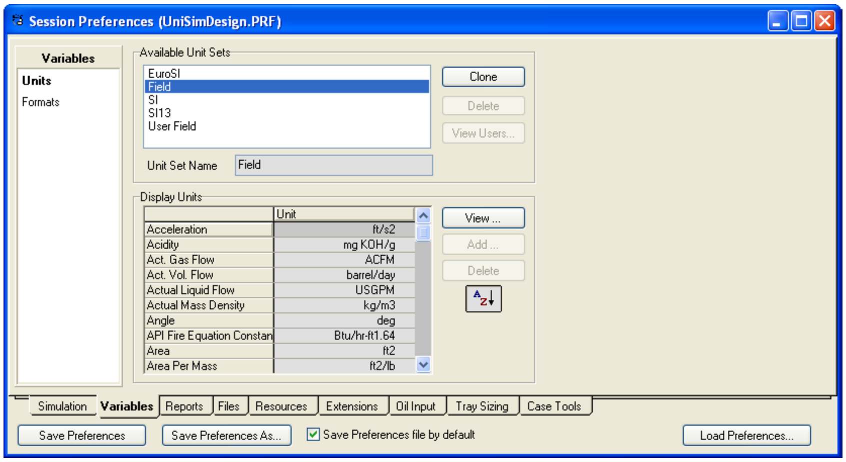
The first step in building the simulation case is choosing a unit set. Since UniSim Design does not allow you to change any of the three default unit sets listed, you will create a new unit set by cloning an existing one. For this example, a new unit set will be made based on the UniSim Design **Field** set, which you will then customize.

To create a new unit set, do the following:

1. In the Session Preferences view, click the **Variables** tab.
2. Select the **Units** page if it is not already selected.

3. In the **Available Unit Sets** group, select **Field** to make it the active set.

Figure 1.4

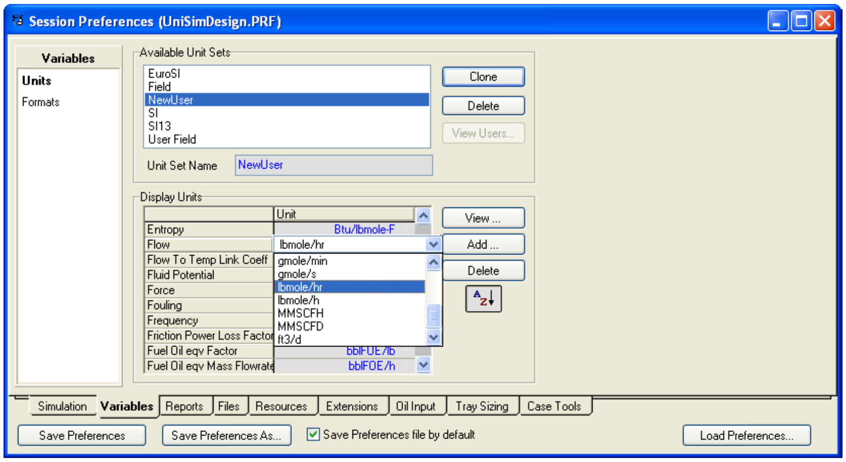


4. Click the **Clone** button. A new unit set named **NewUser** appears. This unit set becomes the currently Available Unit Set.
5. In the **Unit Set Name** field, enter a name for the new unit set.

   You can now change the units for any variable associated with this new unit set.
6. In the Display Units group, scroll down until you find the unit for **Flow**. The default setting is lbmole/hr.

   A more appropriate unit for the Flow is **MMSCFD**.
7. To view the available units for **Flow**, open the drop-down list in the cell beside the **Flow** cell.

Figure 1.5



8. Scroll through the list using either the scroll bar or the arrow keys, and select **MMSCFD**.

   Your new unit set is now defined.

Close icon

9. Click the **Close** icon (in the top right corner) to close the Session Preferences view.

Next, you will start building the simulation case.

1.2.3 Building the Simulation

In building a simulation case UniSim Design split the configuration options into two different environment:

- Basis environment enables you to specify the basic information like components, property package, reactions and so forth associated to the simulation.
- Case environment enables you to specify the streams and operation equipment associated to the simulation, and view the calculated results from the simulation.

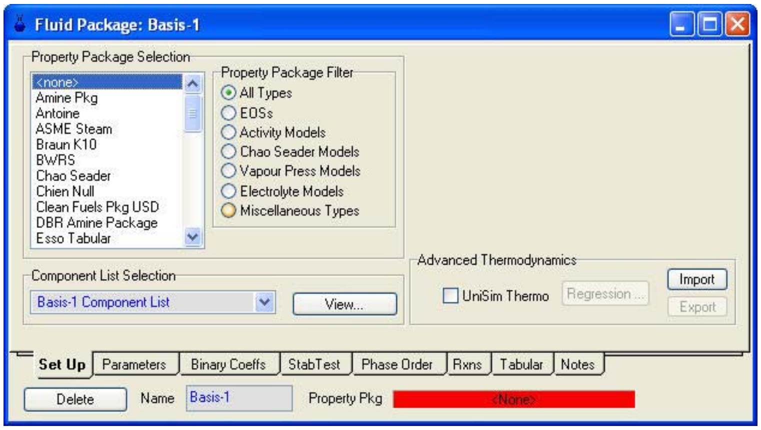
Creating a Fluid Package

The next step is to add a Fluid Package. As a minimum, a Fluid Package contains the components and property method (for example, an Equation of State) UniSim Design will use in its calculations for a particular flowsheet. Depending on what is required in a specific flowsheet, a Fluid Package may also contain other information such as reactions and interaction parameters.

1. On the Simulation Basis Manager view, click the **Fluid Pkgs** tab.
2. Click the **Add** button, and the property view for your new Fluid Package appears.

UniSim Design 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** field at the bottom of the view.

Figure 1.6



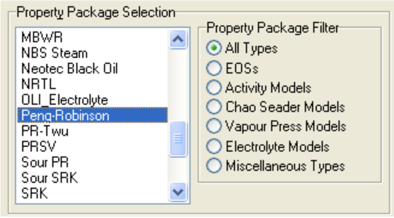
The property view is divided into a number of tabs. Each tab contains the options that enables you to completely define the Fluid Package.

The first step in configuring a Fluid Package is to choose a Property Package on the **Set Up** tab. The current selection is **<none>**.

For this tutorial, you will select the Peng Robinson property package.

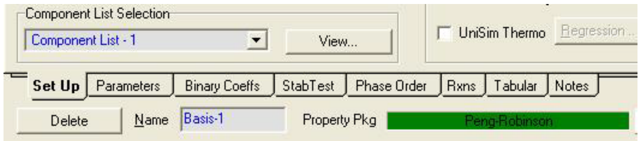
3. Do **one** of the following:
   - Select **<none>** in the Property Package Selection list and type **Peng Robinson**. UniSim Design automatically finds the match to your input.
   - Select **<none>** in the Property Package Selection list and the up and down keys to scroll through the Property Package Selection list until **Peng Robinson** is selected.
   - Use the vertical scroll bar to move up and down the list until **Peng Robinson** becomes visible, then select it.

Figure 1.7



The **Property Pkg** indicator at the bottom of the Fluid Package view now indicates that **Peng Robinson** is the current property package for this Fluid Package. UniSim Design has also automatically created an empty component list to be associated with the Fluid Package.

Figure 1.8

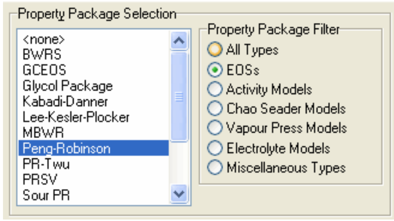


Alternatively, you could have selected the **EOSs** radio button in the **Property Package Filter** group, which filters the list to display only property packages that are Equations of State.

The filter option helps narrow down your search for the **Peng**

Robinson property package, as shown in the figure below.

Figure 1.9



Creating a Component List

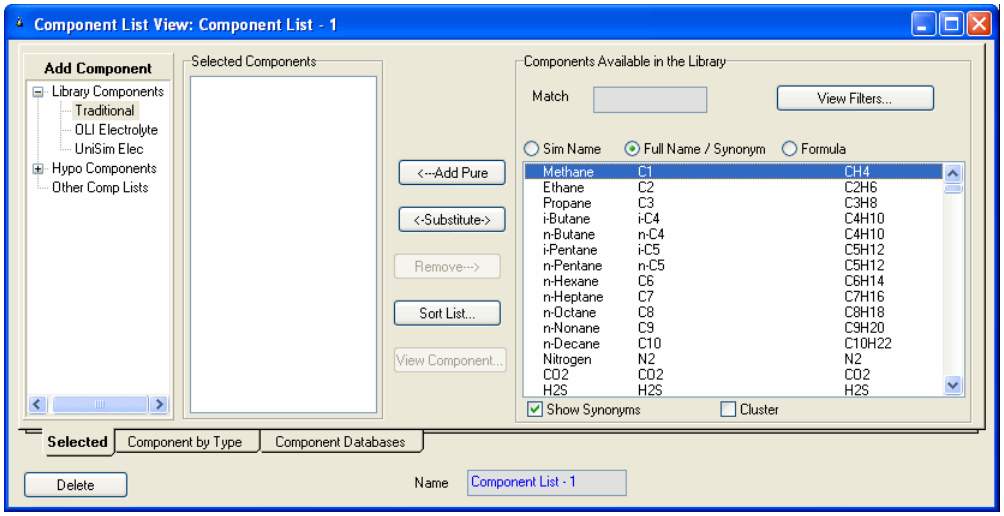
Now that you have selected a property package to be used in the simulation, the next step is to select the components. You can create a list of components using the options on the Components tab of the Simulation Basis Manager view or from the Set Up tab of the Fluid Package view.

In this tutorial, we will create the component list using the option in the Fluid Package view:

1. **In the Set Up tab, select Component List-1 from the Component List Selection drop-down list.**
2. Click the **View** button.

   The Component List View appears.

Figure 1.10



There are a number of ways to select components for your simulation. One method is to use the matching feature. Each

component is listed in three ways on the Selected tab:

Matching Method	Description
Sim Name	The name appearing within the simulation.
Full Name / 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.

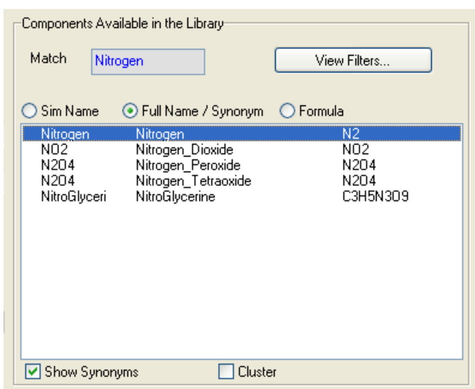
At the top of each of these three columns is a corresponding radio button. Based on the selected radio button, UniSim Design locates the component(s) that best matches the input you type in the **Match** cell.

For this tutorial, you will add the following components: **N2, CO2, C1, C2, C3, i-C4** and **n-C4**.

First, you will add nitrogen using the match feature.

3. Ensure the **Full Name / Synonym** radio button is selected, and the **Show Synonyms** checkbox is checked.
4. Move to the **Match** field by clicking on the field, or by pressing **Alt M**.
5. Type **Nitrogen**. UniSim Design filters as you type and displays only components that match your input.

Figure 1.11



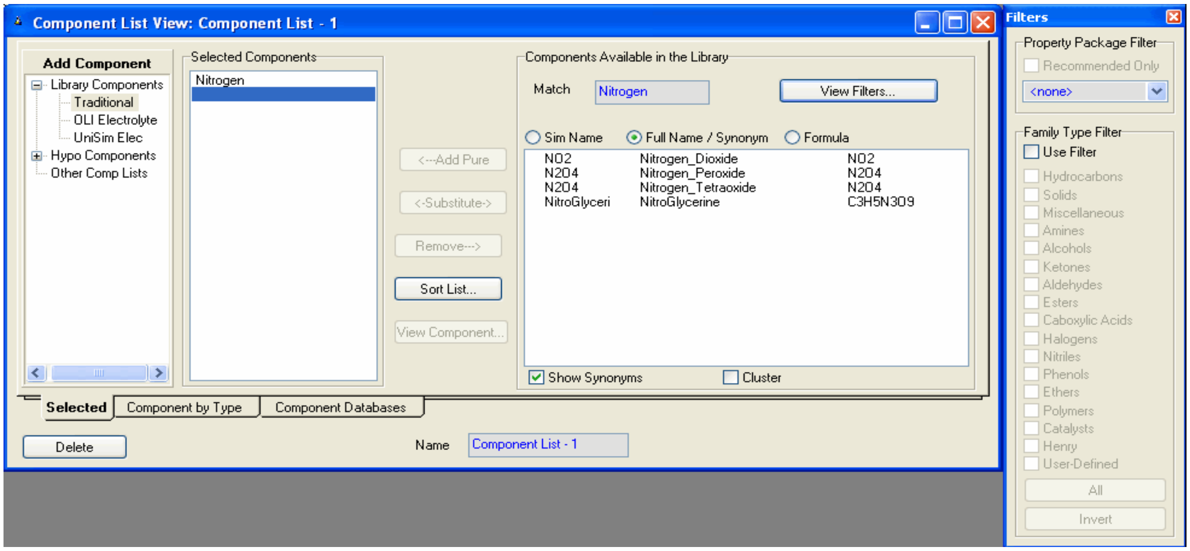
6. With **Nitrogen** selected, add it to the current composition list by doing **one** of the following:
   - Press the **ENTER** key.
   - Click the **Add Pure** button.
   - Double-click on **Nitrogen**.

   In addition to the three match criteria radio buttons, you can also use the **Filters view** to display only those components belonging to certain families.

Next you will add CO2 to the component list using the filter feature.

7. Ensure the Match field is empty by pressing **Alt M** and **DELETE**.
8. Click the **View Filters** button. The Filters view appears as shown in the figure below.

Figure 1.12



9. Select the **Use Filter** checkbox.
10. CO2 does not fit into any of the standard families, so select the **Miscellaneous** checkbox.
11. Scroll down the filtered list until **CO2** becomes visible.
12. Add the **CO2** component to the component list.

    The Match feature remains active when you use a filter, so you could also type **CO2** in the **Match** field to find the component.
13. To add the remaining components **C1** through **n-C4** using the filter, clear the **Miscellaneous** checkbox, and check the **Hydrocarbons** checkbox.

The following shows you a quick way to add components that appear consecutively in the library list:

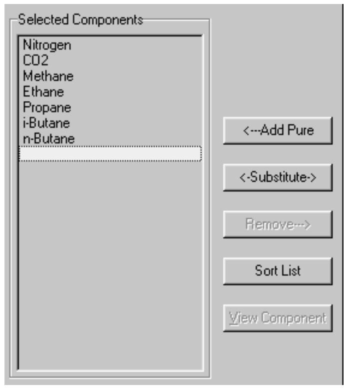
14. Click on the first component in the list (in this case, **C1**).
15. Do **one** of the following:
    - Hold the **SHIFT** key and click on the last component required, in this case n-C4. All components **C1** through **n-C4** will now be selected. Release the **SHIFT** key.
    - Click and hold on **C1**, drag down to **n-C4**, and release the mouse button. **C1** through **n-C4** will be selected.
16. Click the **Add Pure** button. The highlighted components are transferred to the **Selected Components list**.

To select multiple non-consecutive components, use the **CTRL** key.

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

The completed component list appears below.

Figure 1.13

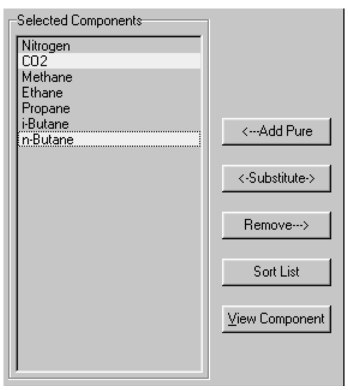


Viewing Component Properties

To view the properties of one or more components, select the component(s) and click the **View Component** button. UniSim Design opens the property view(s) for the component(s) you selected. For example:

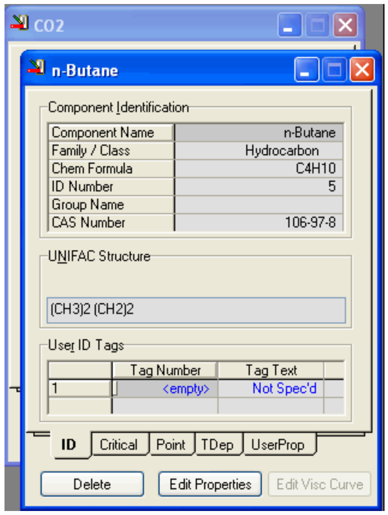
1. Click on **CO2** in the Selected Components list.
2. Press and hold the **CTRL** key.
3. Click on **n-Butane**. The two components should now be selected.
4. Release the **CTRL** key.

Figure 1.14



5. Click the **View Component** button. The property views for the two components appear.

Figure 1.15



See **Chapter 3 - Hypotheticals in the UniSim Design Simulation Basis Guide for more information about cloning library components.**

The Component property view only allows you to view the pure component information. You cannot modify any parameters for a library component, however, UniSim Design allows you to clone a library component as a Hypothetical component, which you can then modify as required.

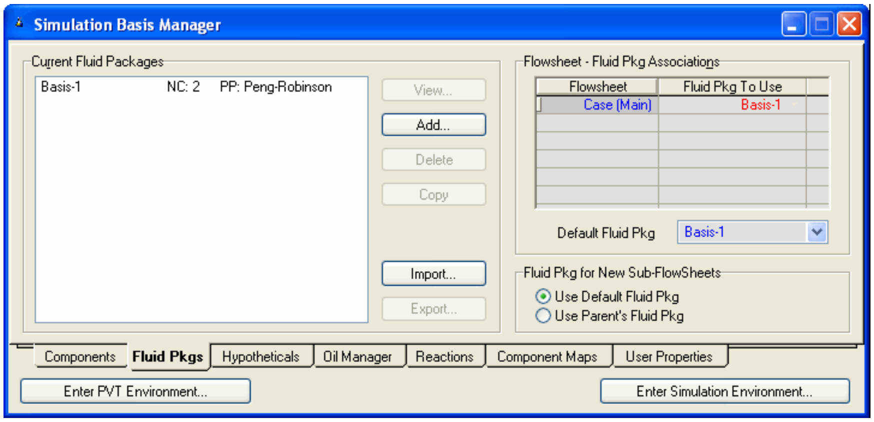
If the Simulation Basis Manager is not visible, select the **Home View** icon from the toolbar.

6. Close both of the component views and the Component List view to return to the Fluid Package view.

   If your project required it, you could continue to add information such as interaction parameters and reactions to the Fluid Package. For the purposes of this tutorial, however, the Fluid Package is now completely defined.

7. Close the Fluid Package view to return to the **Simulation Basis Manager view**.

Figure 1.16



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

8. 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 view.
   - Click the **Enter Simulation Environment** icon on the tool bar.

Enter Simulation Environment icon

1.2.4 Entering the Simulation Environment

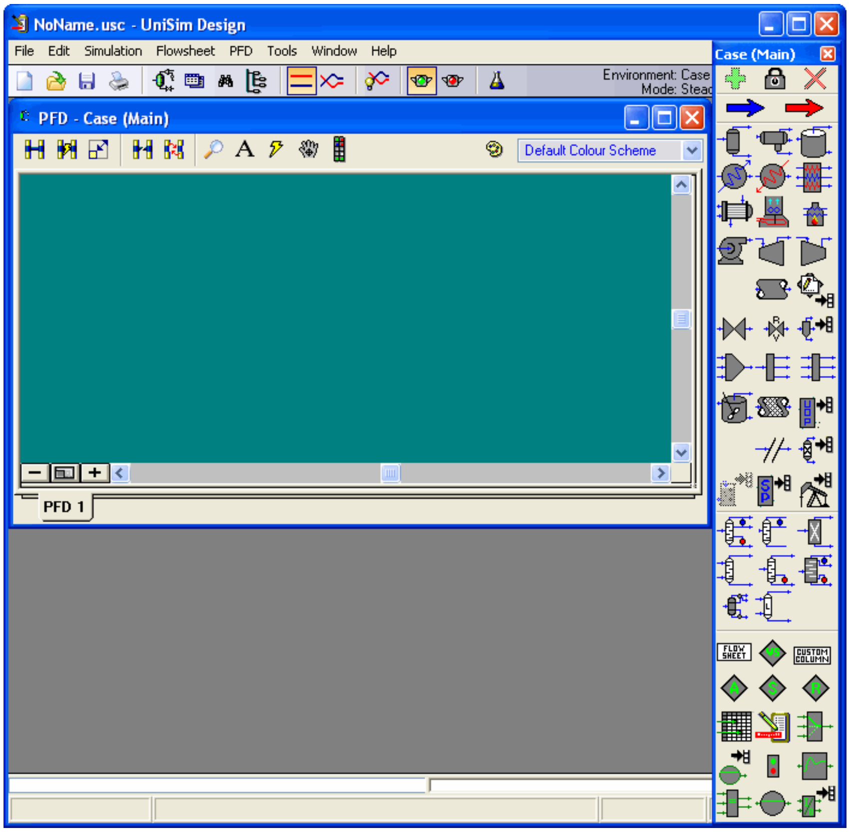
When you enter the Simulation environment, the initial view that appears depends on your current Session Preferences setting for the Initial Build Home View. Three initial views are available:

- PFD
- Workbook
- Summary

Any or all of these can be displayed at any time; however, when you first enter the Simulation environment, only one appears. In this example, the initial Home View is the PFD (UniSim Design default

setting).

Figure 1.17



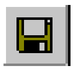
There are several things to note about the Main Simulation environment. In the upper right corner, the Environment has changed from **Basis** to **Case (Main)**. A number of new items are now available in the menu bar and tool bar, and the PFD and Object Palette are open on the Desktop. These latter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

Objects	Description
PFD	The PFD is a graphical representation of the flowsheet topology for a simulation case. The PFD view shows operations and streams and the connections between the objects. You can also attach information tables or annotations to the PFD. By default, the view has a single tab. If required, you can add additional PFD pages to the view to focus in on the different areas of interest.
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 selecting the **Open/Close Object Palette** command from the **Flowsheet** menu.

1. Before proceeding any further, save your case by doing **one** of the

following:

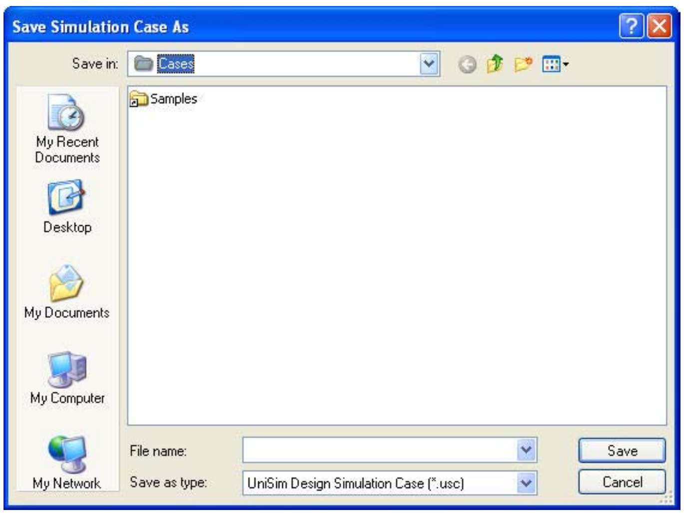
- From the **File** menu, select **Save**.
- Press **CTRL S**.
- Click the **Save** icon on the toolbar.



Save icon

If this is the first time you have saved your case, the Save Simulation Case As view appears.

Figure 1.18



When you choose to open an existing case by clicking the **Open Case** icon  , or by selecting **Open Case** from the File menu, a view similar to the one shown in **Figure 1.18** appears.

The File Filter drop-down list will then allow you to retrieve backup (*.bk*) and HYSIM (*.sim) files and HYSYS®[1] (*.hsc) in addition to standard UniSim Design (*.usc) files.

By default, the File Path is the Cases sub-directory in your UniSim Design directory.

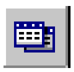
2. In the **File Name** cell, type a name for the case, for example **GASPLANT**. You do not have to enter the ***.usc** extension; UniSim Design automatically adds it for you.
3. Once you have entered a file name, press the **ENTER** key or click the **Save** button.

   UniSim Design saves 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, UniSim Design will ask you for confirmation before over-writing the existing file.

1. HYSYS® is a registered trademark of Aspen Techology.

1.2.5 Using the Workbook

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



Workbook icon

1. Click the **Workbook** icon on the toolbar to access the Workbook

view.

Installing the Feed Streams

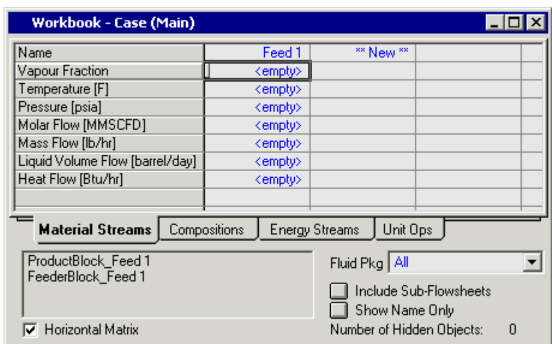
In general, the first action you perform when you enter the Simulation environment is installing one or more feed streams. The following procedure explains how to create a new stream.

UniSim Design accepts blank spaces within a stream or operation name.

1. On the **Material Streams** tab of the Workbook, type the stream name **Feed 1** in the cell labelled **New**, and press **ENTER**.

   UniSim Design will automatically create the new stream with the name defined above. Your Workbook should appear as shown below.

Figure 1.19



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

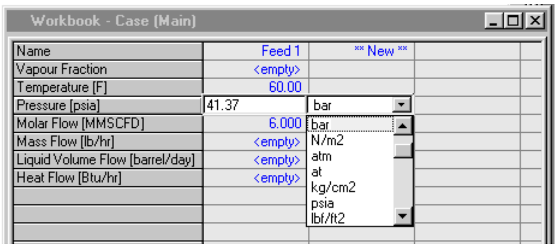
Next you will define the feed conditions.

2. Move to the **Temperature** cell for Feed 1 by clicking it, or by pressing the **DOWN** arrow key.
3. Type **60** in the **Temperature** cell. In the Unit drop-down list, UniSim Design displays the default units for temperature, in this case **F**. This is the correct unit for this exercise.
4. Press the **ENTER** key.

   Your active location should now be the Pressure cell for Feed 1. If you know the stream pressure in another unit besides the default unit of psia, UniSim Design will accept your input in any one of the available different units and automatically convert the supplied value to the default unit for you. For this example, the pressure of Feed 1 is 41.37 bar.

1. In the **Pressure** cell, type **41.37.**
2. Click the  icon in the Unit drop-down list to open the list of units, or press the **SPACE BAR** to move to the Units drop-down list.
3. Either scroll through the list to find **bar**, or begin typing it. UniSim Design will match your input to locate the required unit.

Figure 1.20



4. Once **bar** is selected, press the **ENTER** key.

   UniSim Design will automatically convert the pressure to the default unit, **psia,** and the active selection moves to the Molar Flow cell for Feed 1.

5. In the **Molar Flow** cell, type **6** and press **ENTER**. The default Molar Flow unit is already MMSCFD, so you do not have to modify the units.

Providing Compositional Input

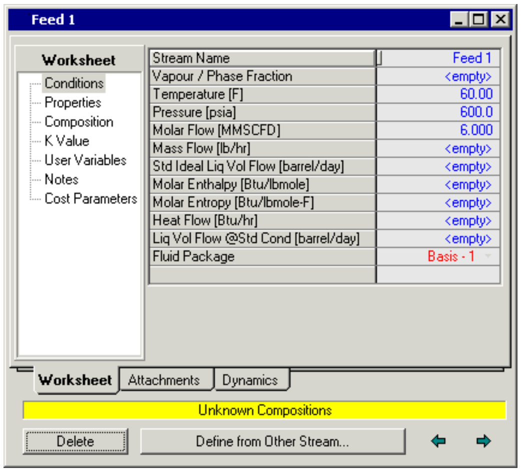
In the previous section you specified the stream conditions in the Workbook property view. Next you will input the composition information in the Stream property view.

1. Close the Workbook view.

   The PFD becomes visible and displays a light blue arrow on it, labeled Feed 1. That arrow is the stream Feed 1 that you just created.

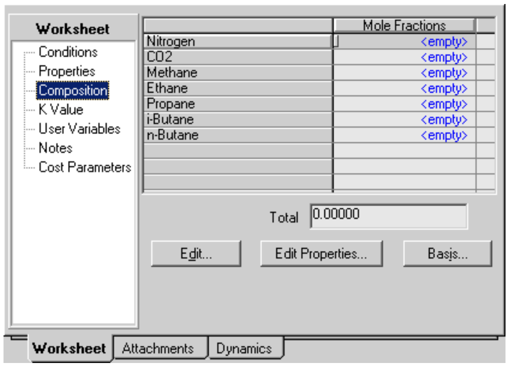
2. Double-click the blue arrow. The Feed 1 view appears.

Figure 1.21



3. Click on the **Composition** page. By default, the components are listed by **Mole Fractions**.

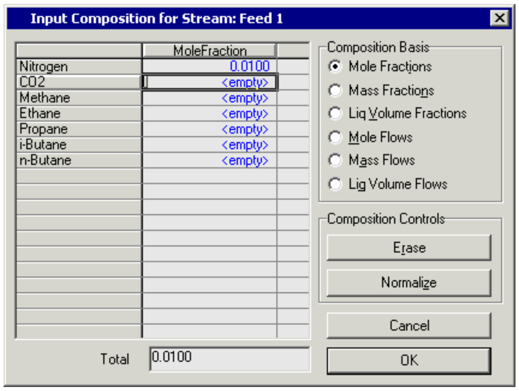
Figure 1.22



4. Click on the **Mole Fractions** cell for the first component, **Nitrogen**.
5. Type **0.01 and** press **ENTER**.

The Input Composition for Stream view appears.

Figure 1.23



This view enables you to access certain features designed to streamline the specification of a stream composition and complete the stream's compositional input.

The following table lists and describes the features available on the Input Composition for Stream view:

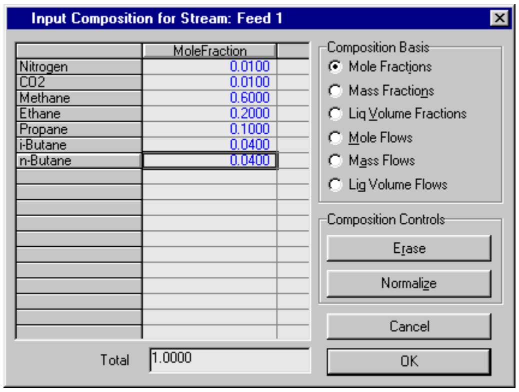
Composition Input	Feature Description
Composition Basis Radio Buttons	Allows you to input the stream composition in some fractional basis other than Mole Fraction, or by component flows, by selecting the appropriate radio button before providing your input.

These are the default colours; yours may appear different depending on your settings on the Colours page on the Resources tab of the Session Preferences view.

Composition Input	Feature Description
Normalizing	The Normalizing feature allows you to enter 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, enter the individual numbers of parts and click the Normalize button. UniSim Design will compute 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, enter the fractions (or the actual flows) for the non-zero components, leaving the others <empty>. Click the Normalize button, and UniSim Design will force 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 will become blue when the composition has been calculated. Three scenarios will 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. Then 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 the OK button. • Input the flows or relative number of parts of all components, including any zero components, then click the OK button.

6. Click on the Mole Fraction cell for **CO2**, type **0.01**, then press **ENTER**.
7. Enter the remaining fractions as shown in the figure below.

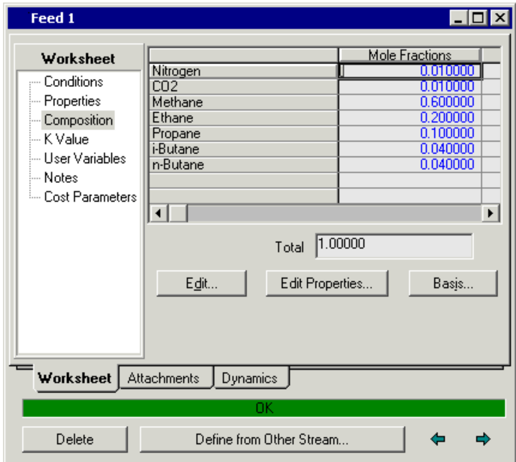
Figure 1.24



When you have entered the fraction of each component the total at the bottom of the view will equal **1.0000**.

8. Click the **OK** button, and UniSim Design accepts the composition. The stream is now completely defined, so UniSim Design flashes it at the conditions given to determine its remaining properties.

Figure 1.25

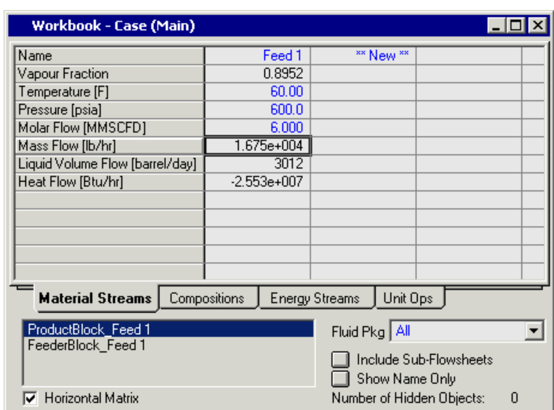


9. Close the Feed 1 property view and access the Workbook view by clicking on the Workbook icon.

10. Ensure that the **Material Streams** tab is active.

The properties of Feed 1 appear below. The values you specified are blue and the calculated values are black.

Figure 1.26



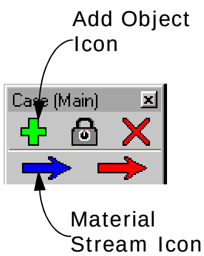
If you want to delete a stream, click on it in the PFD, then press the DELETE key. UniSim Design will ask for confirmation before deleting.

You can also delete the stream using the Delete button on that stream's view.

Alternative Methods for Defining Streams

In addition to the method you just learned, there are several alternative ways to define streams.

1. Access the **Object Palette by** pressing **F4**.
2. 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 on the **Add Object** icon.



   Each of the above four methods creates a new stream and access the property view of the new stream.

   The new stream is named according to the **Automatic Naming** of Flowsheet Objects setting defined in the Session Preferences (Simulation tab, Naming page). UniSim Design names any new material streams with numbers starting at 1 and any new energy streams starting at **100**.

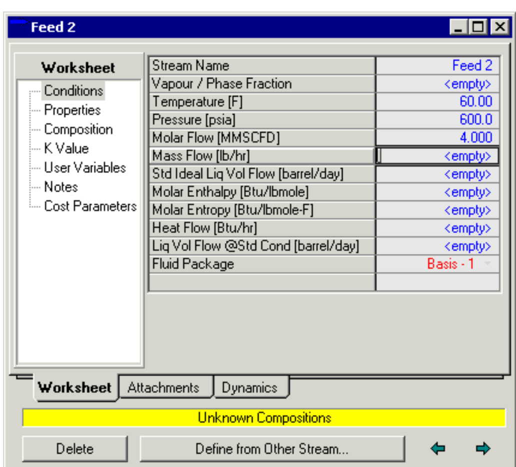
   When you initially access the stream property view, the Conditions page on the **Worksheet** tab is the active page, and **1** appears in the Stream Name cell.

3. In the **Stream Name** cell, replace the name by typing **Feed 2**, then press **ENTER**.

All these variables are in the default units.

4. Enter the following values:
   - Temperature: **60**
   - Pressure: **600**
   - Molar Flow: **4**

Figure 1.27

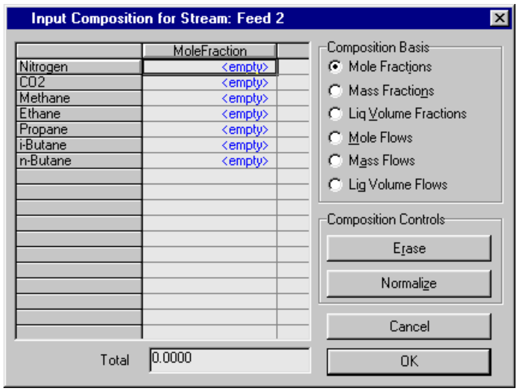


5. Select the **Composition** page and click the **Edit** button.

The Input Composition for Stream view appears.

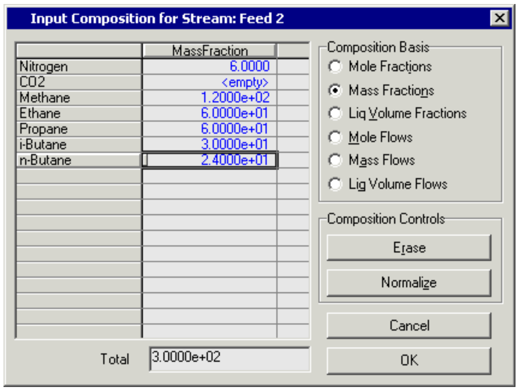
The current Composition Basis setting is the Preferences default. You must enter the stream composition on a mass basis.

Figure 1.28



6. Change the Composition Basis to **Mass Fractions** by selecting the appropriate radio button, or by pressing **ALT N**.
7. Click on the compositional cell for **Nitrogen**, type **6** for the number of parts of this component, then press **ENTER**.
8. Press the **DOWN** arrow key to move to the input cell for **Methane**. Feed 2 does not contain CO2.
9. Input the number of mass parts for the remaining components as shown in the following figure.

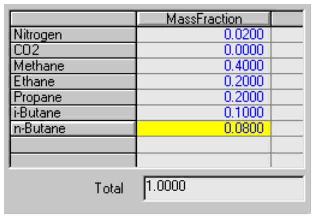
Figure 1.29



10. Click the **Normalize** button once you have entered the parts, and UniSim Design will convert your input to component mass fractions.

For CO2 (the component you left <empty>), the Mass Fraction was automatically forced to zero.

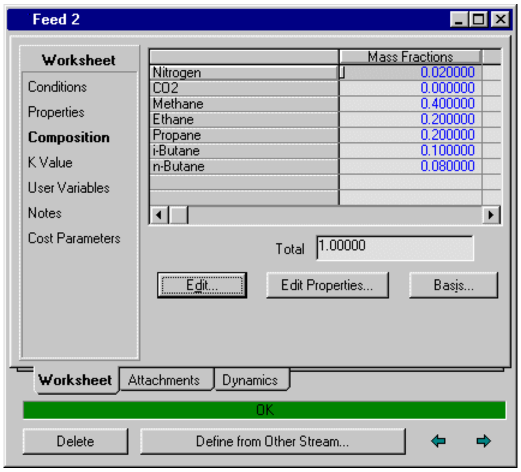
Figure 1.30



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

    UniSim Design performed a flash calculation to determine the unknown properties of **Feed 2**, as indicated by the green OK status in the status bar.

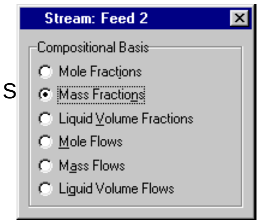
Figure 1.31



For streams with multiple phases, you can view the properties of each phase using the horizontal scroll bar in the table on the property view, or drag and expand the stream property view to see all the phase columns.

To expand the property view, move your cursor over the right border of the view. The cursor becomes a sizing arrow. With the arrow visible, click and drag to the right until the horizontal scroll bar disappears, leaving the entire table visible.

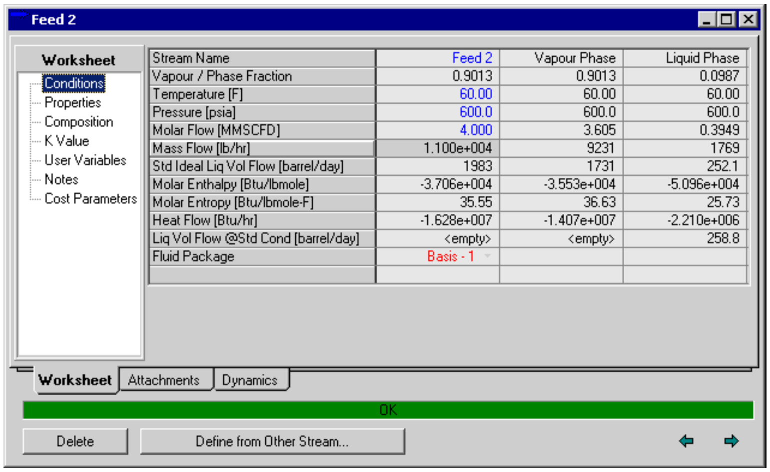
S



The compositions currently appear in Mass Fraction. To change this, click the **Basis** button, then select the appropriate radio button in the Composition Basis group of view that appears.

To view the calculated stream properties, click the **Conditions** page. New or updated information is automatically and instantly transferred among all locations in UniSim Design.

Figure 1.32

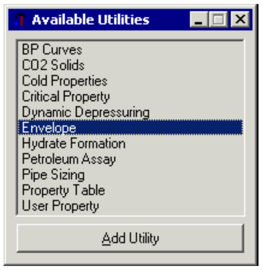


Viewing a Phase Diagram

You can view a phase diagram for any material stream using the UniSim Design Envelope Utility.

1. On the property view for stream Feed 2, click the **Attachments** tab, then select the **Utilities** page.
2. Click the **Create** button to create a phase envelope for the stream. The **Available Utilities** view appears, displaying a list of UniSim Design utilities.
3. Do **one** of the following:
   - Select **Envelope** and click the **Add Utility** button.
   - Double-click on **Envelope**.

Figure 1.33



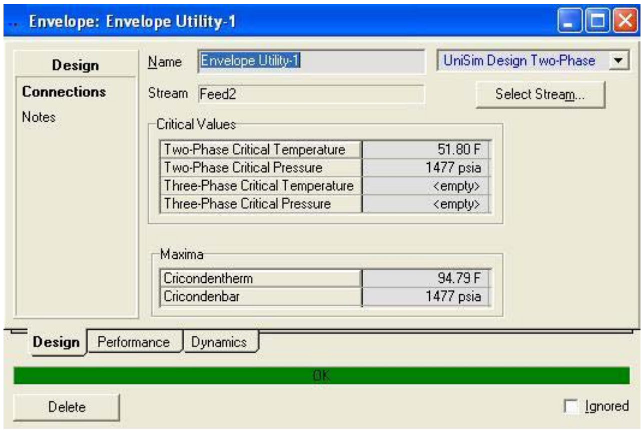
The Envelope Utility view appears. UniSim Design creates and

displays a phase envelope for the stream. Just as with a stream, a Utility has its own property view containing all the information needed to define the utility. Initially, the Connections page of the Design tab appears.

> **A Utility is a separate entity from the stream to which it is attached; if you delete it, the stream will not be affected.**
>
> **Likewise, if you delete the stream, the Utility will remain but will not display any information until you attach another stream using the Select Stream button.**

The Design tab allows you to change the name of the Utility and the stream that it is attached to, and view Critical Values and Maxima.

Figure 1.34

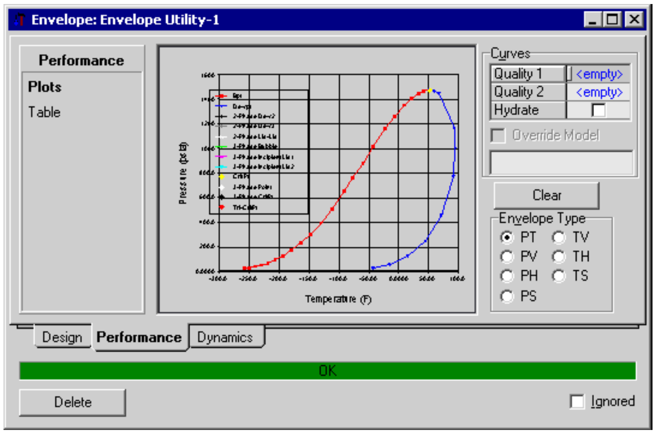


To make the envelope property view more readable, maximize or re-size the view.

4. Click the **Performance** tab, then select the **Plots** page.

   The default **Envelope Type** is **PT**.

Figure 1.35



To view another envelope type, select the appropriate radio button in the Envelope Type group. Depending on the type of envelope selected, you can specify and display Quality curves, Hydrate curves, Isotherms, and Isobars.

To view the data in a tabular format, select the **Table** page.

5. Close the Utility view.

   For more information about defining utilities, refer to **Section 7.27 - Utilities** in the **UniSim Design User Guide**.

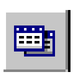
6. Close the Feed 2 view.

1.2.6 Installing Unit Operations

In the last section you defined the feed streams. Now you will install the necessary unit operations for processing the gas.

Installing the Mixer

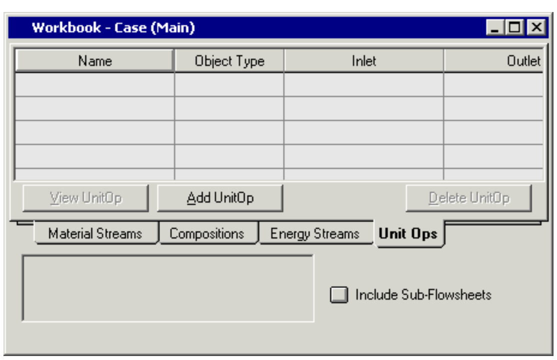
The first operation that you will install is a **Mixer**, used to combine the two feed streams. As with most commands in UniSim Design, installing an operation can be accomplished in a number of ways. One method is through the **Unit Ops** tab of the **Workbook**.



Workbook icon

1. Click the **Workbook** icon to access the Workbook view.
2. Click the **Unit Ops** tab of the Workbook.

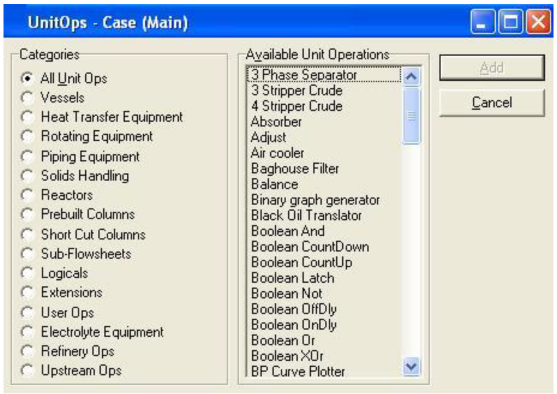
Figure 1.36



3. Click the **Add UnitOp** button.

The **UnitOps** view appears, listing all available unit operations.

Figure 1.37



4. Select **Mixer** by doing one of the following:
   - Click on an operation in the Available Unit Operations list and type **mixer**.
   - Click on an operation in the Available Unit Operations list an press the **DOWN** arrow key to scroll down the list of available operations to Mixer.
   - Scroll down the list using the vertical scroll bar and click on **Mixer**.

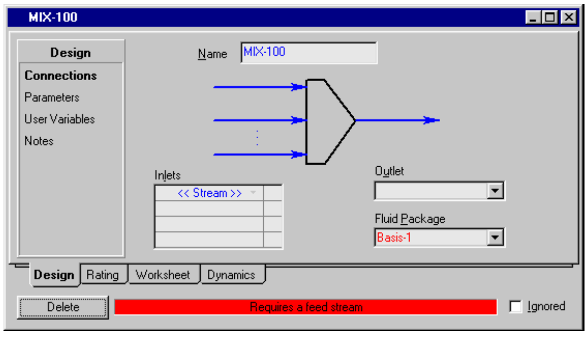
You can also double-click an operation to install it.

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

   You can also use the filters to find and add an operation. For example, select the **Piping Equipment** radio button under Categories. A filtered list containing just piping operations appears in the Available Unit Operations group.

   The Mixer property view appears.

Figure 1.38



As with a stream, a unit operation's property view contains all the information defining the operation, organized in tabs and pages. The four tabs shown for the **Mixer**, namely Design, Rating, Worksheet, and Dynamics, appear in the property view for most

operations. More complex operations have more tabs. UniSim Design provides the default name MIX-100 for the Mixer.

See **Section 12.2.4 - Naming Page** in the **UniSim Design User Guide** for detailed information on setting your Session Preferences.

As with streams, the default naming scheme for unit operations can be changed on the Session Preferences view.

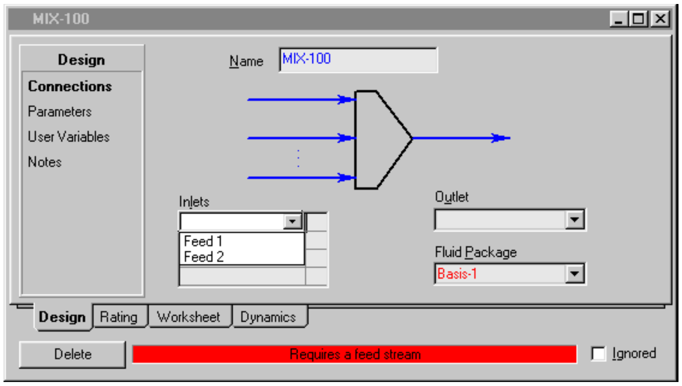
Many operations, such as the Mixer, accept multiple feed streams. Whenever you see a table like the one in the Inlets group, the operation will accept multiple stream connections at that location. When the Inlets table has focus, you can access a drop-down list of available streams.

6. Click the **<<Stream>>** cell.

   The status bar at the bottom of the view shows that the operation requires a feed stream.

7. Open the **<<Stream>>** drop-down list of feeds by clicking on or by pressing the **F2** key and then the **DOWN** arrow key.

Figure 1.39



8. Select **Feed 1** from the list. The stream is added to the list of Inlets, and <<**Stream**>> automatically moves down to a new empty cell.

9. Repeat steps 6-8 to connect the other stream, **Feed 2**.

   The status indicator now displays '**Requires a product stream'**.

Alternatively, you can make the connections by typing the exact stream name in the cell, then pressing **ENTER**.

10. Click in the **Outlet** field.

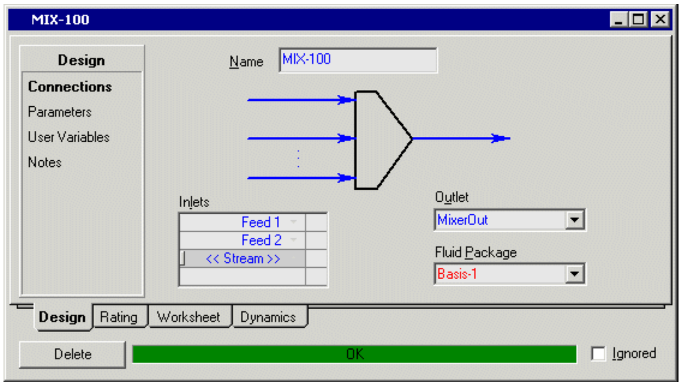
11. Type **MixerOut** in the cell and press **ENTER**.

    UniSim Design recognizes that there is no existing stream named MixerOut, so it will create the new stream with this name.

    The status indicator now displays a green **OK**, indicating that the

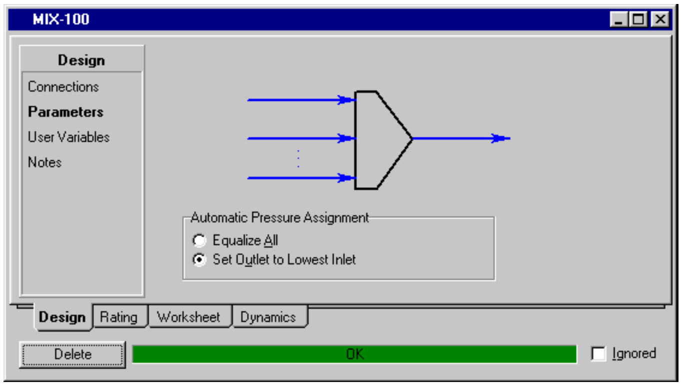
operation and attached streams are completely calculated.

Figure 1.40



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

Figure 1.41

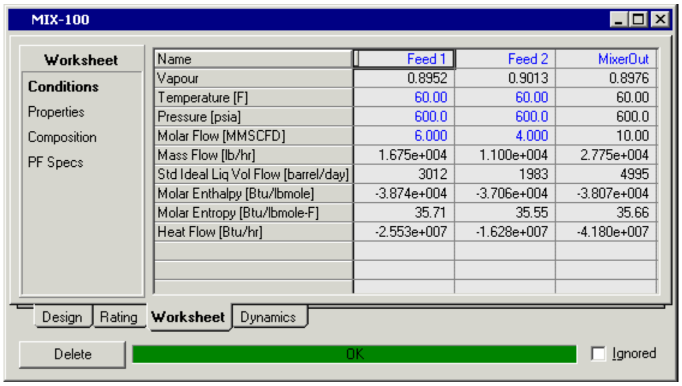


UniSim Design has calculated the outlet stream by combining the two inlets and flashing the mixture at the lowest pressure of the inlet streams. In this case, both inlets have the same pressure (600 psia), so the outlet stream is set to 600 psia.

The Conditions page is a condensed Workbook page, displaying only those streams attached to the selected operation.

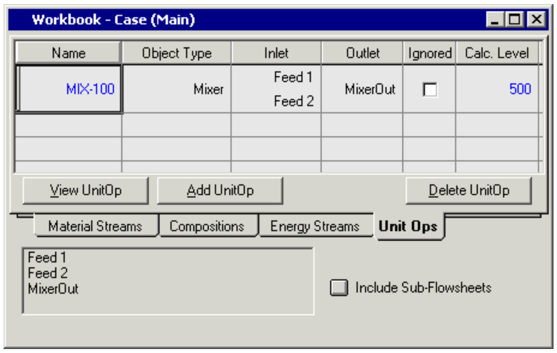
14. To view the calculated outlet stream, click the **Worksheet** tab and select the **Conditions** page.

Figure 1.42



15. Now that the Mixer is completely known, close the view to return to the Workbook. The new operation appears in the table on the **Unit Ops** tab of the Workbook.

Figure 1.43



The table shows the operation Name, its Object Type, the attached streams (Feeds and Products), whether it is Ignored, and its Calculation Level.

When you select an operation in the table and click the **View UnitOp** button, the property view for the selected operation appears. Alternatively, double-clicking on any cell (except Inlet, Outlet, and Ignored) associated with the operation also opens the operation property view.

When any of the **Name**, **Object Type**, **Ignored,** or **Calc**. **Level** cells are active, the box at the bottom of the Workbook displays all streams attached to the current operation. Currently, the Name cell for **MIX-100** has focus, and the box displays the three streams attached to this operation.

You can also open the property view for a stream directly from the **Unit Ops** tab. To open the property view for one of the streams attached to an operation, do **one** of the following:

- Select the operation in the Unit Ops tab and double-click on the stream you want to access in the list at the bottom of the **Workbook view.**
- Double-click on the **Inlet** or **Outlet** cell of the operation. The property view for the first listed feed or product stream appears.

Installing the Inlet Separator

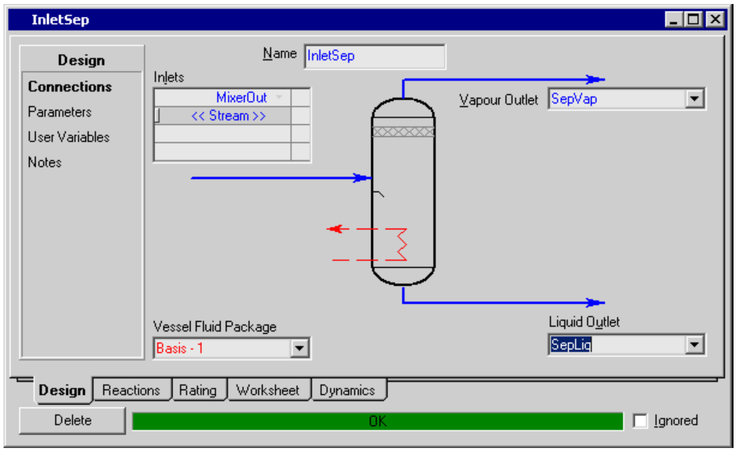
Next you will install and define the inlet separator, which splits the two-phase MixerOut stream into its vapour and liquid phases.

1. In the Workbook property view, click the **Unit Ops** tab.
2. Click the **Add UnitOp** button. The UnitOps view appears. You can also access the Unit Ops view by pressing **F12**.
3. In the Categories group, select the **Vessels** radio button.
4. In the list of Available Unit Operations, select **Separator**.
5. Click the **Add** button. The Separator property view appears, displaying the **Connections** page on the **Design** tab.
6. In the **Name** cell, change the name to **InletSep** and press **ENTER**.
7. Move to the Inlets list by clicking on the **<< Stream>>** cell, or by pressing **ALT L**.
8. Open the drop-down list of available feed streams.
9. Select the stream **MixerOut** by doing one of the following:
   - Click on the stream name in the drop-down list.
   - Press the **DOWN** arrow key to highlight the stream name and press **ENTER**.
10. Move to the **Vapour Outlet** cell by pressing **ALT V**.
11. Create the vapour outlet stream by typing **SepVap** and pressing **ENTER**.

An Energy stream could be attached to heat or cool the vessel contents. For this tutorial, however, the energy stream is not required.

12. Click on the **Liquid Outlet** cell, type the name **SepLiq**, and press **ENTER**. The completed Connections page appears as shown in the following figure.

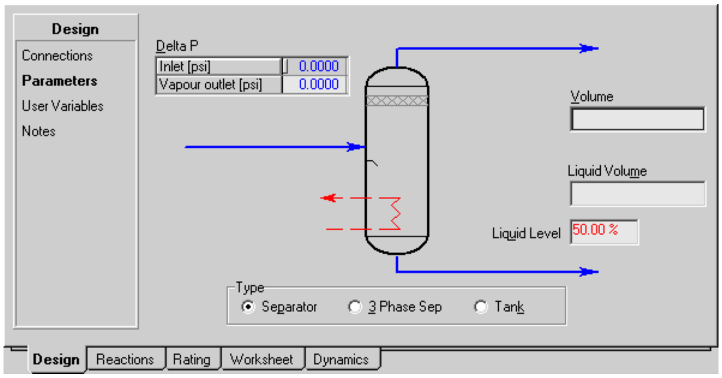
Figure 1.44



The Volume, Liquid Volume, and Liquid Level default values generally apply only to vessels operating in dynamic mode or with reactions attached.

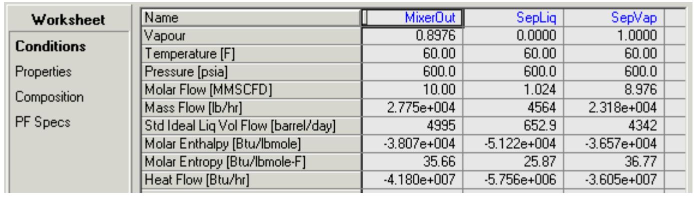
13. Select the **Parameters** page. The current default values for Delta P, Volume, Liquid Volume, and Liquid Level are acceptable.

Figure 1.45



14. To view the calculated outlet stream data, click the **Worksheet** tab, then select the **Conditions** page. The table appearing on this page is shown below.

Figure 1.46



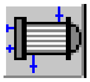
Name	MixerOut	SepLiq	SepVap
Vapour	0.8976	0.0000	1.0000
Temperature [F]	60.00	60.00	60.00
Pressure [psia]	600.0	600.0	600.0
Molar Flow [MMSCFD]	10.00	1.024	8.976
Mass Flow [lb/hr]	2.775e+004	4564	2.318e+004
Std Ideal Liq Vol Flow [barrel/day]	4995	652.9	4342
Molar Enthalpy [Btu/lbmole]	-3.807e+004	-5.122e+004	-3.657e+004
Molar Entropy [Btu/lbmole-F]	35.66	25.87	36.77
Heat Flow [Btu/hr]	-4.180e+007	-5.756e+006	-3.605e+007

15. When finished, click the **Close** icon to close the separator property view.

Installing the Heat Exchanger

Next, you will install the gas/gas exchanger.

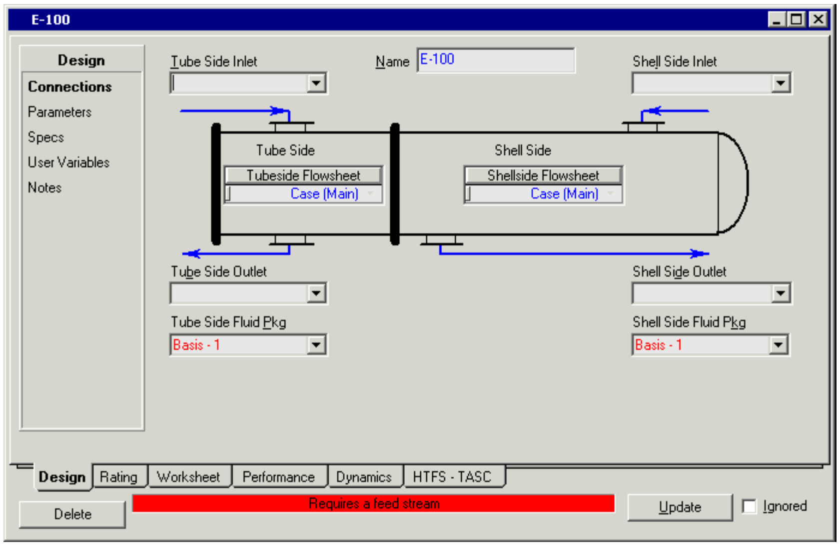
1. Access the Object Palette by pressing **F4**.
2. On the Object Palette, double-click the **Heat Exchanger** icon.



Heat Exchanger Icon

   The **Heat Exchanger** property view appears.

Figure 1.47



   The **Connections** page on the **Design** tab is active.

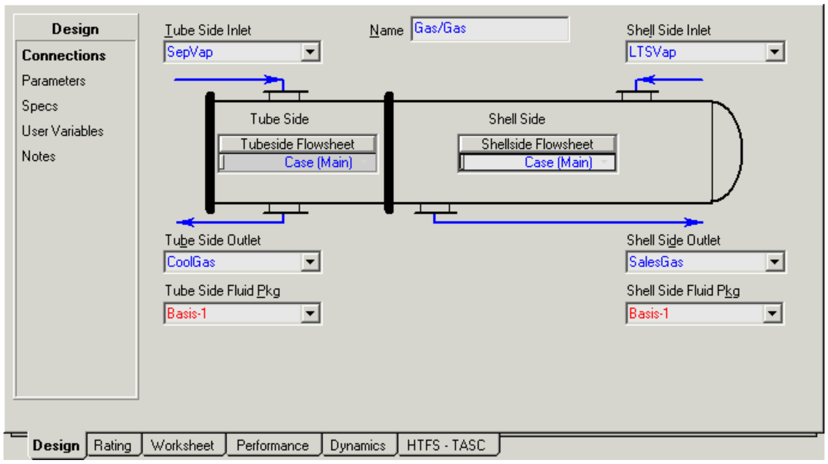
3. In the **Name** field, change the operation **name** from its default E-100 to **Gas/Gas**.

You will have to create all streams except **SepVap**, which is an existing stream that can be selected from the **Tube Side Inlet** drop-down list.

Create the new streams by selecting the appropriate input field, typing the name, then pressing **ENTER**.

4. Attach the Inlet and Outlet streams as shown below, using the methods learned in the previous sections.

Figure 1.48

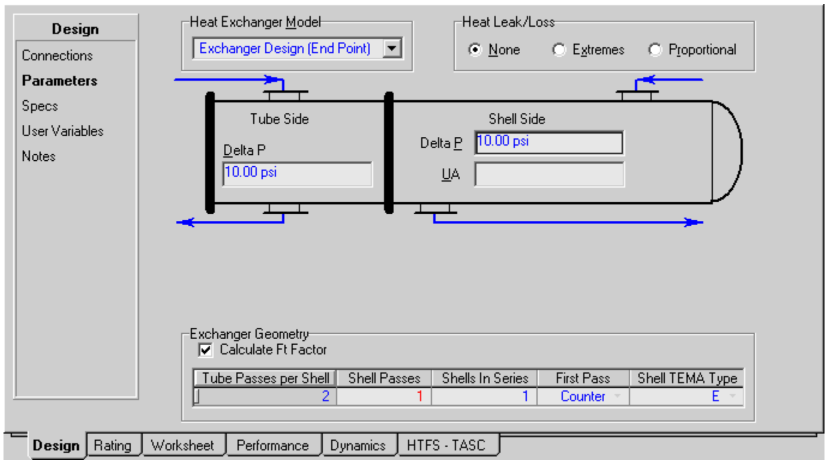


5. Click the **Parameters** page.

   The **Exchanger Design (End Point)** is the acceptable default setting for the Heat Exchanger Model for this tutorial.

6. Enter a pressure drop of **10 psi** for both the **Tube Side Delta P** and **Shell Side Delta P**.

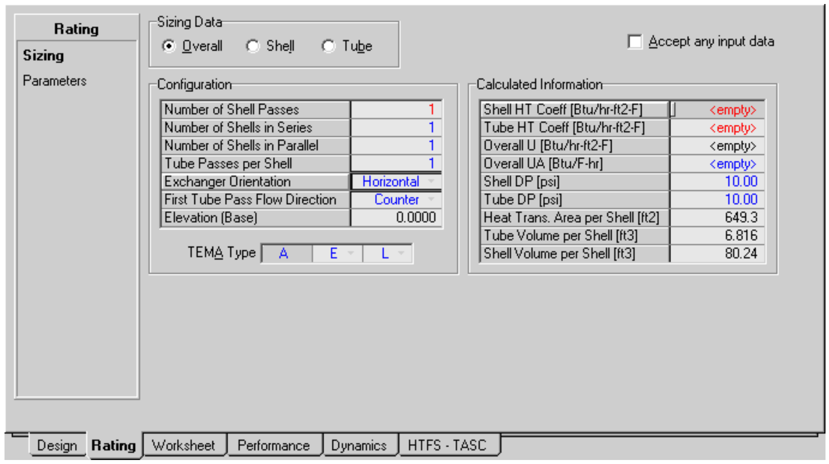
Figure 1.49



7. Click the **Rating** tab, then select the **Sizing** page.

8. In the Configuration group, click in the **Tube Passes per Shell** cell and change the value to **1**, to model Counter Current Flow.

Figure 1.50

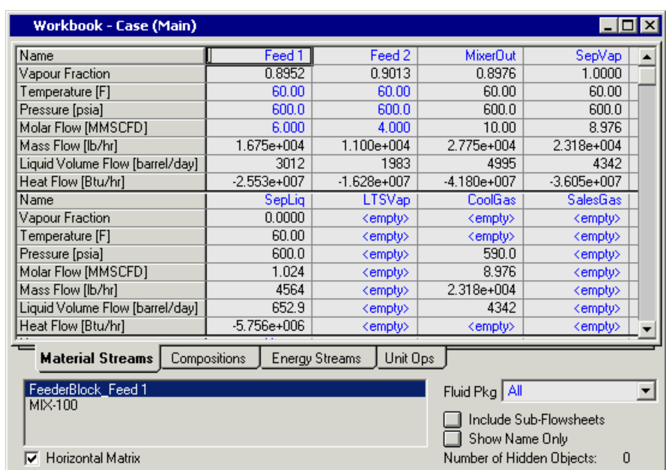


9. A warning appears to remind you that the number of tube passes must be an even multiple of the shell passes. Click the **OK** button.

10. Close the **Heat Exchanger** property view to return to the **Workbook view**.

11. Click the **Material Streams** tab of the **Workbook**.

Figure 1.51



Notice how partial information is passed (for stream CoolGas) throughout the flowsheet. UniSim Design always calculates as many properties as possible for the streams based on the available information.

Stream **CoolGas** has not yet been flashed, as its temperature is unknown. The **CoolGas** stream is flashed later when a temperature approach is specified for the **Gas/Gas** heat exchanger.

1.2.7 Using 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

There are several ways to open the property view for an operation directly from the **Workbook**. In addition to using the **Unit Ops tab**, you can use the following method:

Any utilities attached to the stream with the Workbook active also appears in (and are accessible through) this list.

1. Click one of the Workbook stream tabs (Material Streams, Compositions, or Energy Streams).

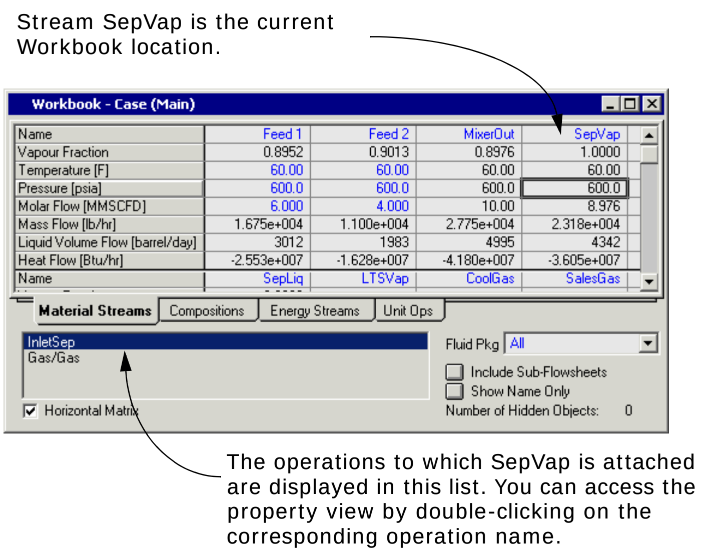
   The list at the bottom of the Workbook view displays the operations to which the selected stream is attached.

2. Click on any cell associated with the stream **SepVap**.

   The list at the bottom displays the names of the two operations, **InletSep** and **Gas/Gas**, to which this stream is attached.

3. To access the property view for either of these operations, double-click on the operation name.

Figure 1.52



Adding a Tab to the Workbook

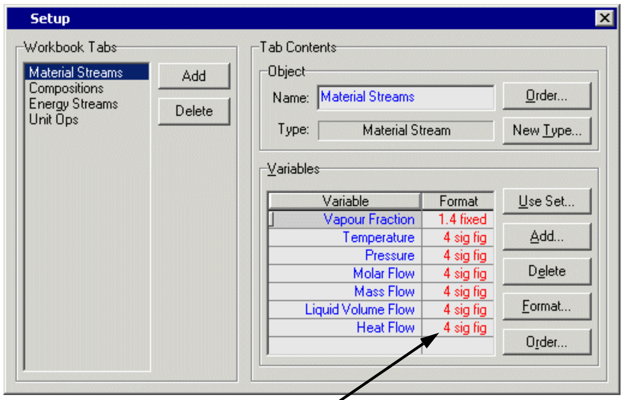
When the **Workbook** has focus, the **Workbook** item appears in the UniSim Design menu bar. This allows you to customize the **Workbook** to display specific information.

In this section 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, select **Setup**.
   - Right-click the Material Streams tab in the Workbook, then select **Setup** from the object inspect menu that appears.

   The Workbook Setup view appears.

Figure 1.53



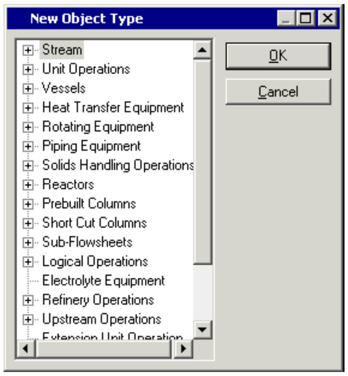
Currently, all variables are displayed with four significant figures. You can change the display format or precision of any Workbook variables by clicking the **Format** button.

   The four existing tabs are listed in the **Workbook** Pages group. When you add a new tab, it will be inserted **before** the highlighted tab (currently **Material Streams**).

2. In the **Workbook** Tabs group list, select the **Compositions** tab.

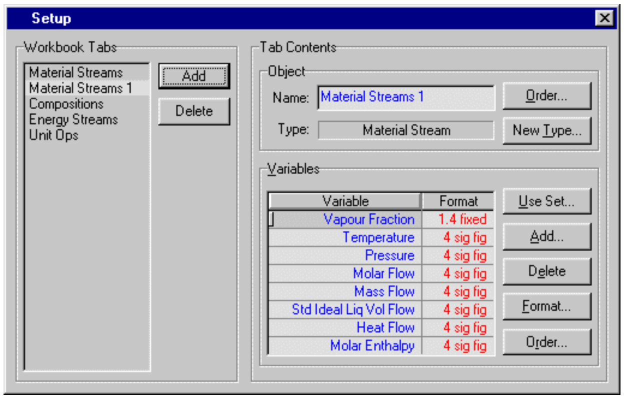
3. In the Workbook Tabs group, click the **Add** button. The New Object Type view appears.

Figure 1.54



4. Click the **+** icon beside **Stream** to expand the tree branch into Material Stream and Energy Streams.
5. Select the **Material Stream** and click the **OK** button. You will return to the **Setup** view, and the new tab appears in the list after the existing **Material Streams** tab.

Figure 1.55

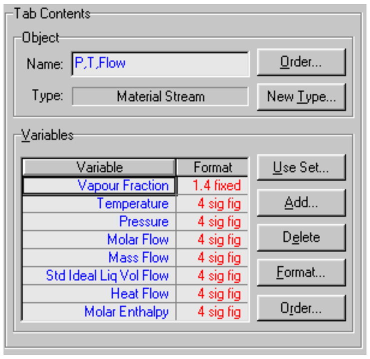


6. In the Object group, click in the **Name** cell and change the name for the new tab from the default **Material Streams 1** to **P,T,Flow** to better describe the tab contents.

   Next you will customize the tab by removing the irrelevant variables.

7. In the Variables group, select the first variable, **Vapour Fraction**.

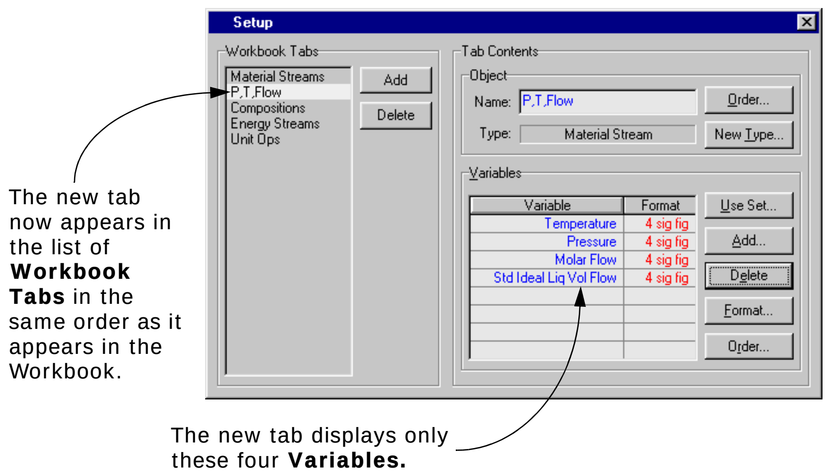
Figure 1.56



8. Press and hold the **CTRL** key.
9. Click on the following variables: **Mass Flow**, **Heat Flow, and Molar Enthalpy**. Four variables are now selected.
10. Release the **CTRL** key.
11. Click the **Delete** button. The variables are removed from the list. The finished Setup appears below.

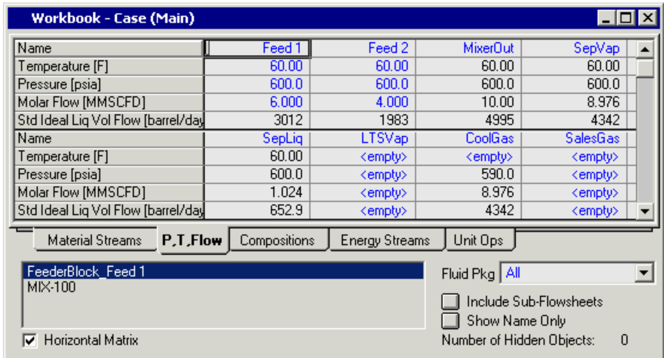
Deleting variables removes them from the current **Workbook** tab **only**. If you want to remove variables from another tab, you must edit each tab individually.

Figure 1.57

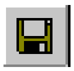


12. Close the Setup view to return to the Workbook view and check the new tab.

Figure 1.58



13. At this point, save your case by doing **one** of the following:



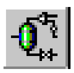
Save Icon

- Click the **Save** icon on the toolbar.
- Select **Save** from the **File** menu.
- Press **CTRL S**.

1.2.8 Using the PFD

The PFD is the other home view used in the Simulation environment. To open the PFD:

1. Do **one** of the following:



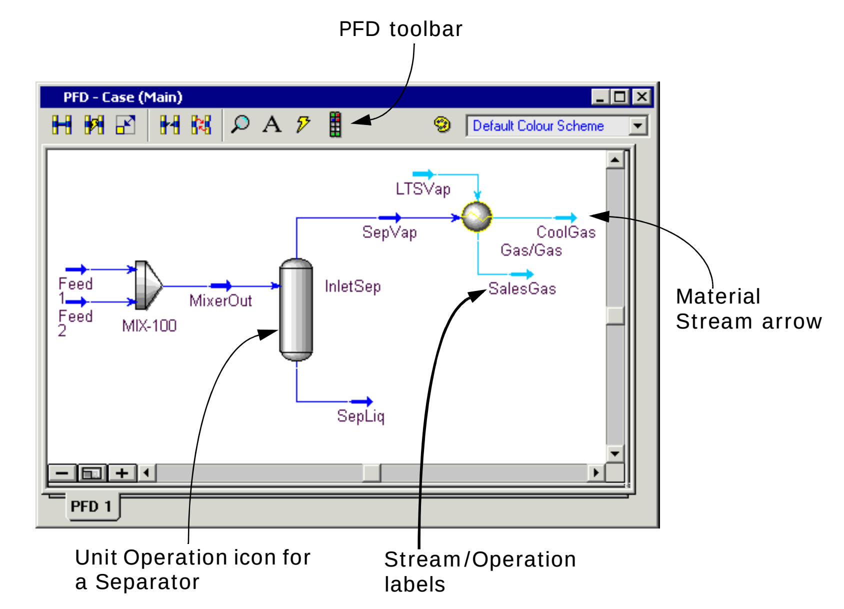
PFD Icon

- Click the **PFD** icon on the toolbar.
- Press **CTRL P** or from the **Tools** menu select **PFDs**. The Select PFD view appears. Select the PFD you want to access from the list and click the **View** button.

The current tutorial PFD view appears as shown in the figure below,

with all streams and unit operations visible.

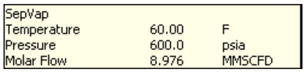
Figure 1.59



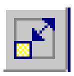
If the streams or operations are not all visible, select **Auto Position All** from the **PFD** menu. UniSim Design now displays all streams and operations, arranging them in a logical manner.

The **PFD** menu option appears in the UniSim Design menu bar whenever the PFD is active.

As a graphic 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 or 'icon'. A stream icon is an arrow pointing in the direction of flow, while an operation icon is a graphic representation of the actual physical operation. The object name or 'label' appears near each icon.

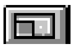


Fly-by Information

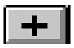


Size Mode Icon

Zoom Out 25%



Display Entire PFD



Zoom In

Like any other non-modal view, the PFD view can be re-sized by clicking and dragging anywhere on the outside border. Other functions you can perform while the PFD is active include the following:

- Access commands and features from the PFD tool bar.
- Open the property view for an object by double-clicking on 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.
- Change an icon's size by clicking the **Size Mode** icon, clicking on the icon you want to resize, then clicking and dragging the sizing "handles" that appear.

- Accessing 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 that particular object.
- Zoom in and out or display the entire flowsheet in the PFD window by clicking the zoom buttons at the bottom left corner of the PFD view.

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

Calculation Status

Before proceeding, you will examine a feature of the PFD which allows you to trace the calculation status of the objects in your flowsheet. If you recall, the status indicator at the bottom of the property view for a stream or operation displayed three different states for the object:

Keep in mind that these are the UniSim Design 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 appears.
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 where the outlet stream temperature is unknown. The status indicator is yellow, and an appropriate warning message appears.
Green Status	The stream or operation is completely defined and solved. The status indicator is green, and an OK message appears.

When you are working in the PFD, the streams and operations are also colour-coded to indicate their calculation status. The mixer and inlet separator are completely calculated, so they have a black outline. For the heat exchanger Gas/Gas, however, the conditions of the tube side outlet and both shell side streams are unknown, so the exchanger has a yellow outline indicating its unsolved status.

The icons for all streams installed to this point are dark blue except for the Heat Exchanger shell-side streams LTSVap and SalesGas, and tube-side outlet CoolGas.

A similar 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 indicates an energy stream with a known duty, while a purple icon indicates an unknown duty.

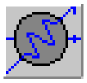
Installing the Chiller

In the next step you will install a chiller, which will be modeled as a Cooler. The operation is installed using the Object Palette the PFD.

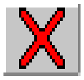
Adding the Chiller to the PFD

1. Press **F4** to access the Object Palette

   The Chiller will be added to the right of the Gas/Gas, so make some empty space available in the PFD by scrolling to the right using the horizontal scroll bar.



Cooler icon



Cancel icon

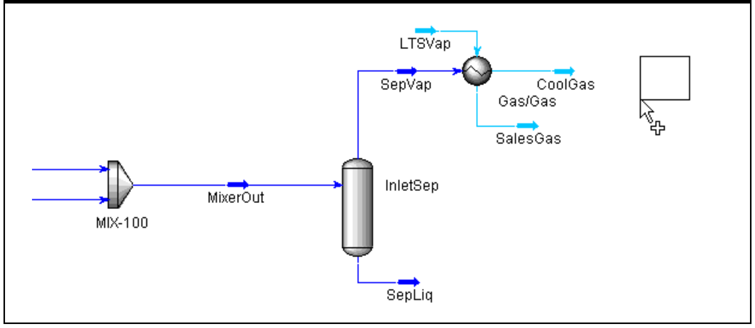
2. Click the **Cooler** icon on the Object Palette.

   If you click the wrong button, click the **Cancel** icon.

3. Position the cursor over the PFD.

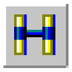
   The cursor changes to a special cursor with a **+** symbol attached to it. A frame attached to the cursor is used to indicate the location of the operation icon.

Figure 1.60



4. Click on the PFD where you want to **drop** the Cooler.

   UniSim Design creates a new Cooler with a default name, E-100. The Cooler has a red status (and colour), indicating that it requires feed and product streams.



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** icon again.

You can temporarily toggle between Attach and Move mode by holding down the **CTRL** key.

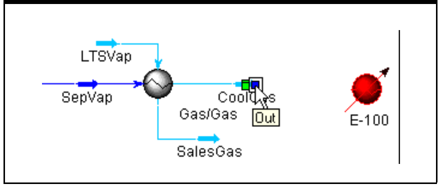
Connecting the Chiller

1. Click the **Attach Mode** icon on the PFD toolbar to enter Attach

mode.

2. Position the cursor over the right end of the **CoolGas** stream icon.

Figure 1.61



A small transparent box appears at the cursor tip. Through the transparent box, you can see a square connection point, and a pop-up description attached to the cursor tail. The pop-up Out indicates which part of the stream is available for connection, in this case the stream outlet.

3. With the pop-up Out visible, click and hold.

   The transparent box becomes solid black, indicating that you are beginning a connection.

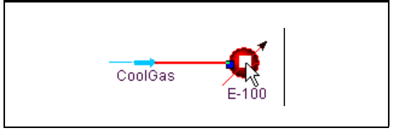
4. Move the cursor toward the left (inlet) side of the Cooler.

   A trailing line appears between the CoolGas stream icon and the cursor, and a connection point appears at the Cooler inlet.

5. Place the cursor near the connection point, and the trailing line snaps to that point.

   Also, a solid white box appears at the cursor tip, indicating an acceptable end point for the connection.

Figure 1.62



6. Release the left mouse button, and the connection is made to the connection point at the Cooler inlet.

Adding Outlet and Energy Streams

1. Position the cursor over the right end of the Cooler icon.

   The connection point and pop-up Product appears.

2. With the pop-up visible, left-click and hold.

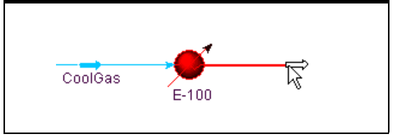
   The transparent box again becomes solid black.

3. Move the cursor to the right of the Cooler.

   A white stream icon appears with a trailing line attached to the

Cooler outlet.

Figure 1.63



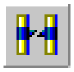
The stream icon indicates that a new stream will be created after the next step is completed.

4. With the white stream icon visible, release the left mouse button.

   UniSim Design creates a new stream with the default name **1**.

If you make an incorrect connection:

1. Click the **Break Connection** icon on the PFD toolbar.

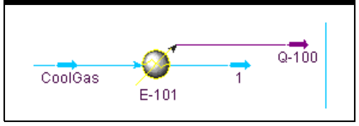


2. Move the cursor over the stream line connecting the two icons. A checkmark attached to the cursor appears, indicating an available connection to break.
3. Click once to break the connection.

5. Repeat steps 1-4 to create the Cooler energy stream, originating the connection from the arrowhead on the Cooler icon.

   The new stream is automatically named Q-100. The Cooler has yellow (warning) status, indicating that all necessary connections have been made but the attached streams are not entirely known.

Figure 1.64



6. Click the **Attach Mode** icon again to return to Move mode.

Defining the Material and Energy Streams

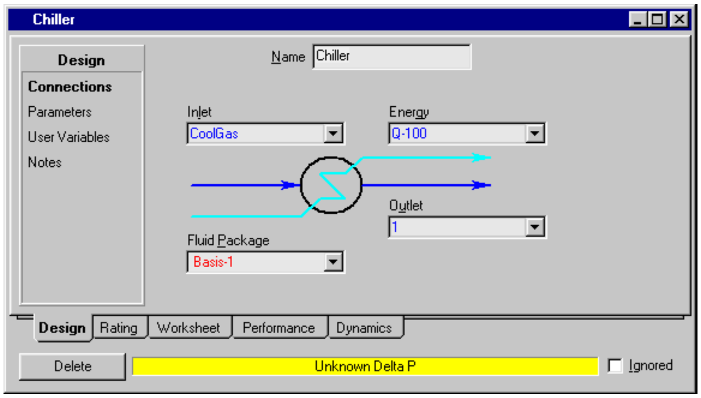
The Cooler material streams and the energy stream are unknown at this point, so they are light blue and purple, respectively.

1. Double-click the **Cooler** icon to open its property view.

   On the **Connections** page, the names of the Inlet, Outlet, and Energy streams that you recently attached appear in the appropriate cells.

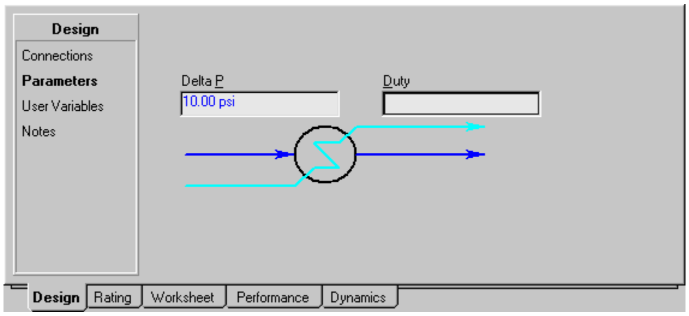
2. In the **Name** field, change the operation name to **Chiller**.

Figure 1.65



3. Select the **Parameters** page.
4. In the **Delta P** field, specify a pressure drop of **10 psi**.

Figure 1.66



5. Close the cooler view.

   At this point, the Chiller has two degrees of freedom; one of these will be exhausted when UniSim Design flashes the CoolGas stream after the exchanger temperature approach is specified.

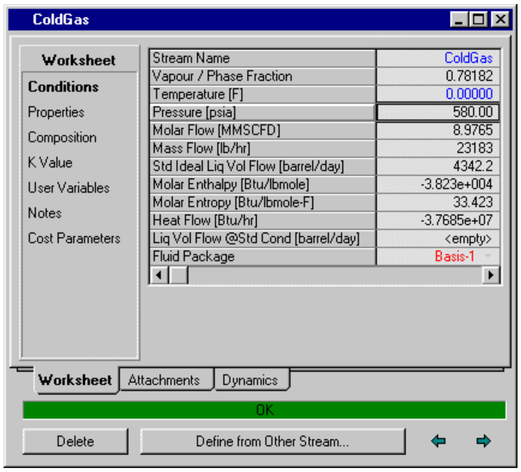
   To use the remaining degree of freedom, either the Chiller outlet temperature or the amount of duty in the Chiller energy stream must be specified. The amount of chilling duty which is available is unknown, so you will provide an initial guess of 0^{o}F for the Chiller outlet temperature. Later, this temperature can be adjusted to provide the desired sales gas dew point temperature.

6. Double-click on the outlet stream icon (**1**) to open its property view.
7. In the **Name** field, change the name to **ColdGas**.
8. In the **Temperature** field, specify a temperature of **0^{o}F**.

   The remaining degree of freedom for this stream has now been

used, so UniSim Design flashes ColdGas to determine its remaining properties.

Figure 1.67



9. Close the ColdGas view and return to the PFD view.

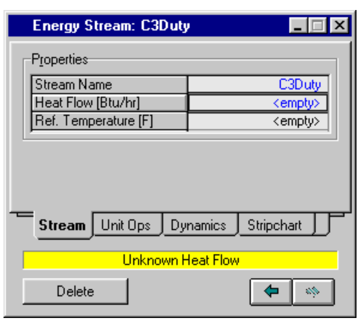
   The Chiller still has yellow status, because the temperature of the CoolGas stream is unknown.

10. Double-click the energy stream icon **(Q-100)** to open its property view.

    The required chilling duty (in the Heat Flow cell) is calculated by UniSim Design when the Heat Exchanger temperature approach is specified in a later section.

11. Rename the energy stream **C3Duty** and close the view.

Figure 1.68

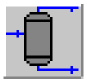


Installing the LTS

Now that the chiller has been installed, the next step is to install the low-temperature separator (LTS) to separate the gas and condensed

liquids in the ColdGas stream.

Adding and Connecting the LTS

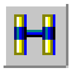


Separator icon

1. Make some empty space available to the right of the Chiller using the horizontal scroll bar.
2. Position the cursor over the **Separator** icon on the Object Palette.
3. Right-click, hold, and drag the cursor over the PFD to the right of the Chiller.

   The cursor changes to a special “bulls-eye” cursor. A frame attached to the bulls-eye cursor indicates the location of the operation icon.
4. Release the right mouse button to **drop** the Separator onto the PFD.

   A new Separator appears with the default name V-100.



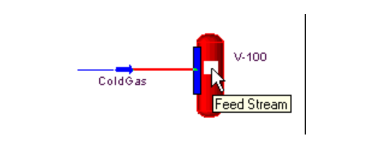
5. Click the **Attach Mode** icon on the PFD tool bar.
6. Position the cursor over the right end of the ColdGas stream icon. The connection point and pop-up Out appears.
7. With the pop-up visible, left-click, hold, and drag the cursor toward the left (inlet) side of the Separator.

   Multiple connection points appear at the Separator inlet.

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

8. Place the cursor near the inlet area of the Separator. A solid white box appears at the cursor tip.

Figure 1.69



9. Release the mouse button and the connection is made.

Adding Connections

The Separator has two outlet streams, liquid and vapour. The vapour outlet stream LTSVap, which is the shell side inlet stream for Gas/Gas, has already been created. The liquid outlet will be a new stream.

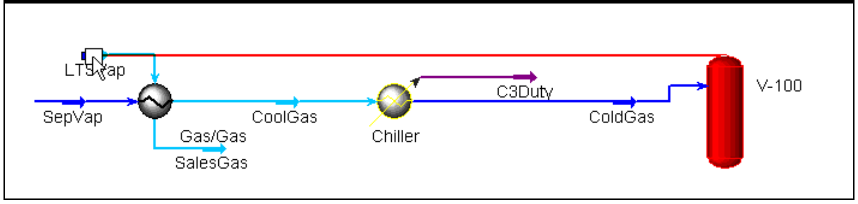
1. In the PFD, position the cursor over the top of the Separator icon.

   The connection point and pop-up Vapour Product appears.
2. With the pop-up visible, left-click and hold.
3. Drag the cursor to the LTSVap stream icon.

   A solid white box appears when you move over the connection

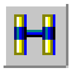
point.

Figure 1.70



4. Release the mouse button, and the connection is made.
5. Position the cursor over the bottom of the Separator icon. The connection point and pop-up Liquid Product appears.
6. With the pop-up visible, left-click and hold.
7. Move the cursor to the right of the Separator.

   A white arrow stream icon appears with a trailing line attached to the Separator liquid outlet.
8. With the stream icon visible, release the mouse button. UniSim Design creates a new stream with the default name **1**.

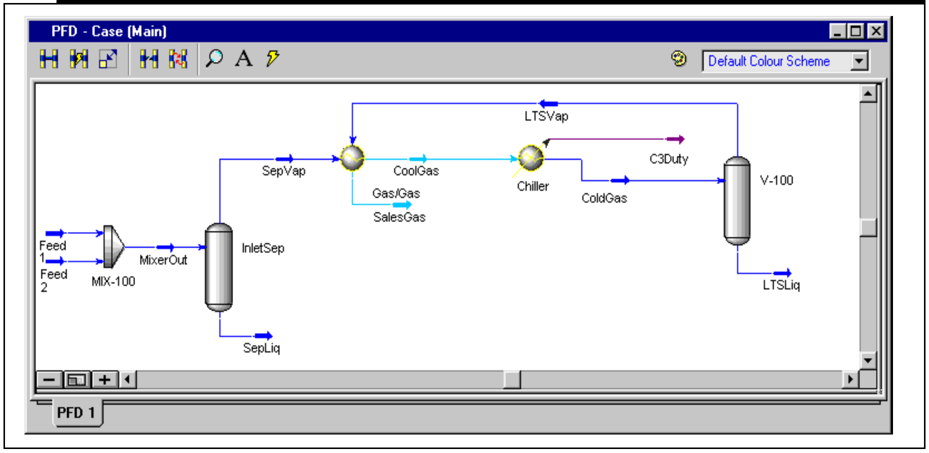


Attach Mode icon

9. Click the **Attach Mode** icon to leave Attach mode.
10. Double-click on the stream icon 1 to open its property view.
11. In the **Stream Name** cell, type **LTSLiq**, then press **ENTER**.
12. Close the LTSLiq stream property view.
13. Select **Auto Position All** from the **PFD** menu.

    Your PFD should appear similar to the one shown below.

Figure 1.71



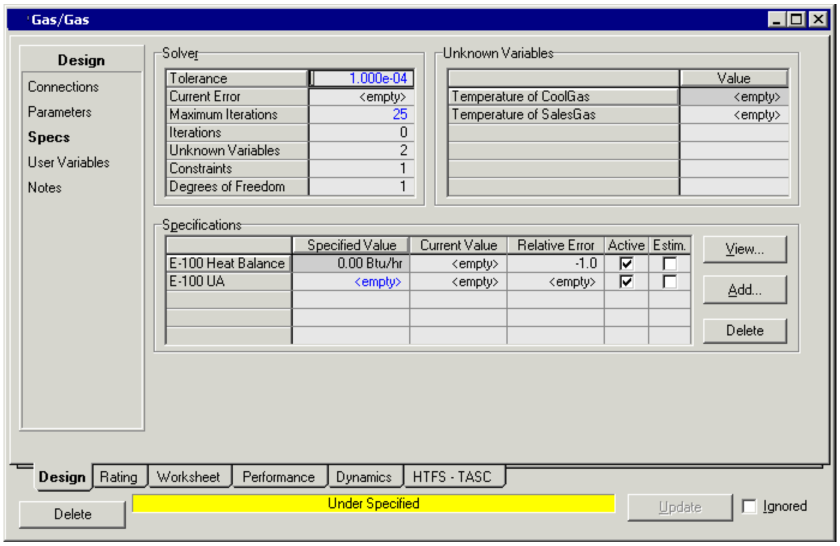
Streams LTSVap and LTSLiq are now known, as shown by the change in their PFD colour from light blue to dark blue.

14. Double-click the icon for the new Separator (V-100) to open its property view.
15. In the **Name** field, change the name to **LTS**.
16. Close the LTS property view.

At this point, the outlet streams from heat exchanger Gas/Gas are still unknown.

17. Double-click on the Gas/Gas icon to open the exchanger property view.
18. Click the **Design** tab and select the **Specs** page.

Figure 1.72



The **Specs** page allows you to input specifications for the Heat Exchanger and view its calculation status. The Solver group on this page shows that there are two Unknown Variables and the Number of Constraints is 1, so the remaining Degrees of Freedom is 1. UniSim Design provides two default constraints in the Specifications group, although only one has a value:

Specification	Description
Heat Balance	The tube side and shell side duties must be equal, so the heat balance must be zero (0).
UA	This is the product of the overall heat transfer coefficient (U) and the area available for heat exchange (A). UniSim Design does not provide a default UA value, so it is unknown at this point. It will be calculated by UniSim Design when another constraint is provided.

Adding a Heat Exchanger Specification

To exhaust the remaining degree of freedom, a 10^{o}F minimum temperature approach to the hot side inlet of the exchanger will be specified.

1. In the Specifications group, click the **Add** button.

   The ExchSpec (Exchanger Specification) view appears.

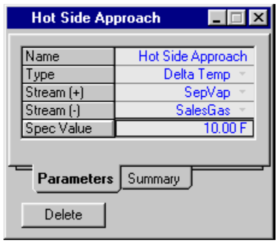
2. In the **Name** cell, change the name to **Hot Side Approach**.

   The default specification in the **Type** cell is **Delta Temp**, which allows you to specify a temperature difference between two streams. The **Stream (+)** and **Stream (-)** cells correspond to the warmer and cooler streams, respectively.

3. In the **Stream (+)** cell, select **SepVap** from the drop-down list.
4. In the **Stream (-)** cell, select **SalesGas** from the drop-down list.
5. In the **Spec Value** cell, enter **10°F**.

   The view should appear as shown in the following figure.

Figure 1.73

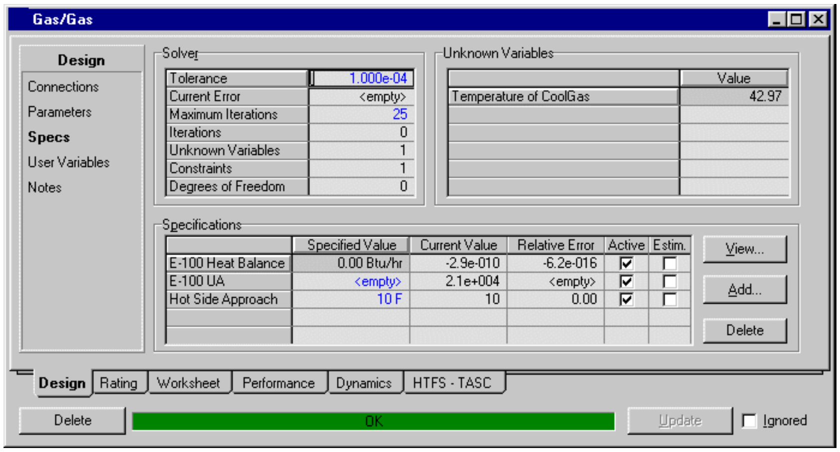


UniSim Design will converge on both specifications and the unknown streams will be flashed.

6. Close the specification view to return to the Gas/Gas property view.

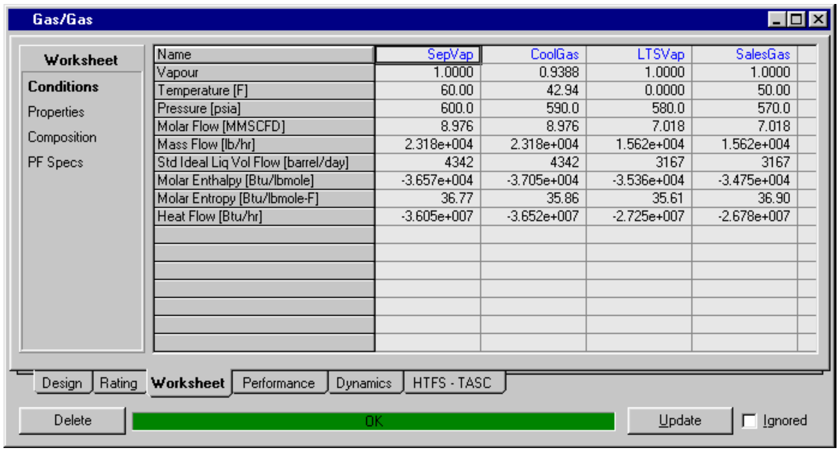
   The new specification appears in the Specifications group on the **Specs** page.

Figure 1.74



7. Click the **Worksheet** tab, then select the **Conditions** page to view the calculated stream properties.

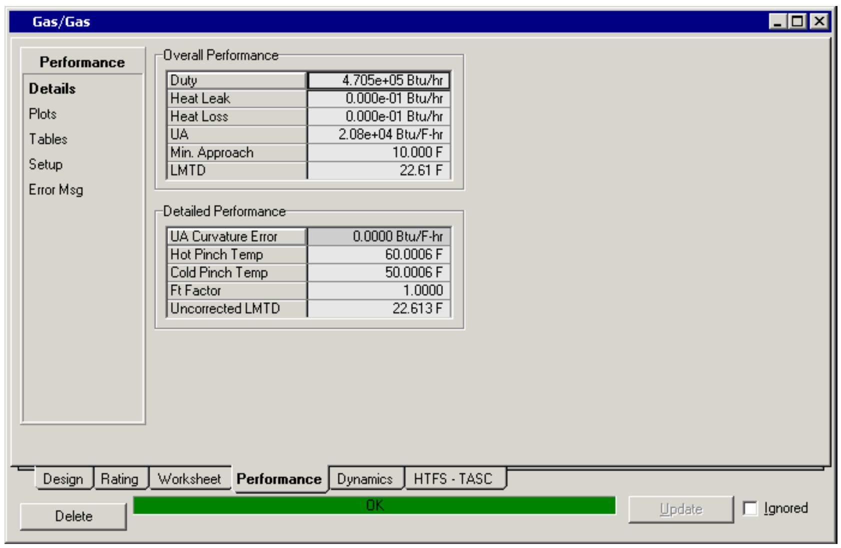
Figure 1.75



Using the **10^{o}F** approach, UniSim Design calculates the temperature of CoolGas as **42.9^{o}F**. All streams in the flowsheet are now completely known.

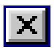
8. Click the **Performance** tab, then select the **Details** page, where UniSim Design displays the Overall Performance and Detailed Performance.

Figure 1.76



Two parameters of interest are the UA and LMTD (logarithmic mean temperature difference), which UniSim Design has calculated as

2.08e4 Btu/F-hr and **22.6°F**, respectively.



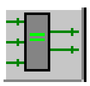
Close icon

9. When you are finished reviewing the results, click the **Close** icon to leave the Gas/Gas property view.

Checking the Sales Gas Dew Point

The next step is to check the SalesGas stream to see if it meets a dew point temperature specification. This is to ensure no liquids form in the transmission line. A typical pipeline dew point specification is 15**°F** at **800 psia**, which will be used for this example.

You can test the current dew point by creating a stream with a composition identical to SalesGas, specifying the dew point pressure, and having UniSim Design flash the new stream to calculate its dew point temperature. To do this you will install a Balance operation.

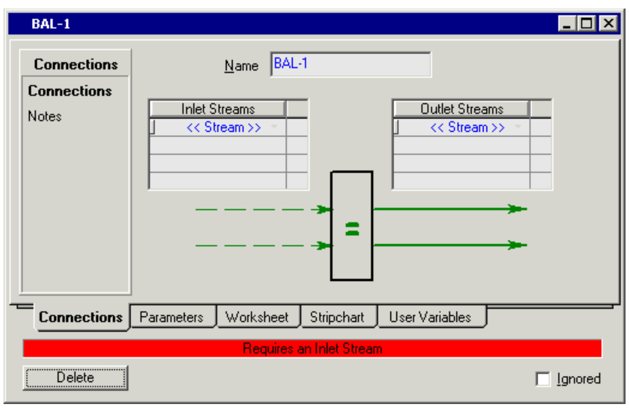


Balance icon

1. Double-click the **Balance** icon on the Object Palette.

   The property view for the new operation appears.

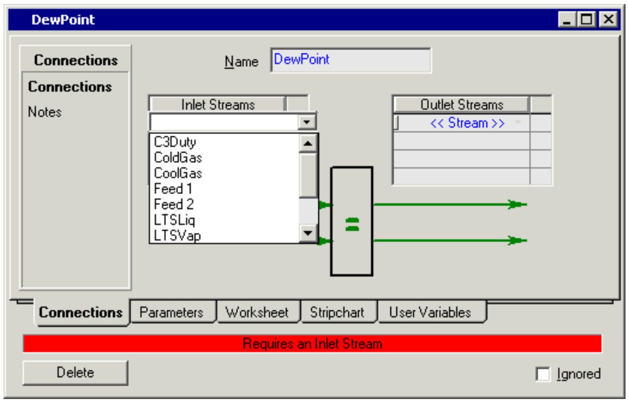
Figure 1.77



2. In the **Name** field, type **DewPoint**, then press **ENTER**.
3. Click in the <<**Stream**>> cell in the Inlet Streams table.

4. Open the drop-down list of available streams and select **SalesGas**.

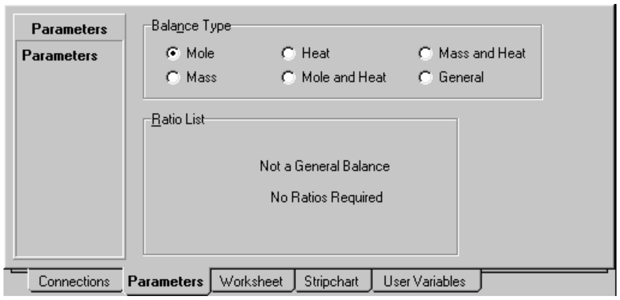
Figure 1.78



5. Click in the <<**Stream**>> cell in the Outlet Streams table.
6. Create the outlet stream by typing **SalesDP**, then press **ENTER**.
7. Click the **Parameters** tab.
8. In the Balance Type group, select the **Mole** radio button.

Changes made to the vapour fraction, temperature or pressure of stream SalesDP will not affect the rest of the flowsheet. However, changes which affect SalesGas will cause SalesDP to be re-calculated because of the molar balance between these two streams.

Figure 1.79



9. Click the **Worksheet** tab.

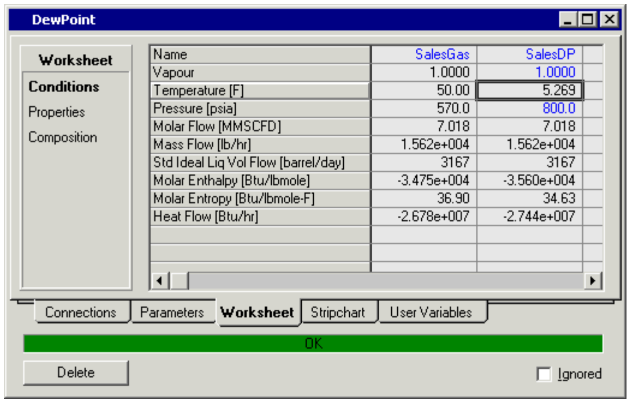
   The vapour fraction and pressure of SalesDP can now be specified, and UniSim Design will perform a flash calculation to determine the unknown temperature.

10. In the SalesDP column, **Vapour** cell, enter **1.0**.
11. In the **Pressure** cell, enter **800 psia**.

    UniSim Design flashes the stream at these conditions, returning a dew point Temperature of **5.27°F**, which is well within the pipeline

of 15°F.

Figure 1.80

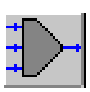


12. Close the DewPoint view to return to the PFD.

    When UniSim Design created the Balance and new stream, their icons were probably placed in the far right of the PFD. If you like, you can click and drag the Balance and SalesDP icons to a more appropriate location, such as immediately to the right of the SalesGas stream.

Installing the Second Mixer

In this section you will install a second mixer, which is used to combine the two liquid streams, SepLiq and LTSLiq, into a single feed for the Distillation Column.



Mixer icon

1. In the PFD, make some empty space available to the right of the LTS using the horizontal scroll bar.
2. Click the **Mixer** button on the Object Palette.
3. In the PFD, position the cursor to the right of the LTSLiq stream icon.
4. Click to **drop** the Mixer onto the PFD.

   A new Mixer named MIX-101 appears.
5. Press and hold the **CTRL** key to temporarily enable **Attach** mode while you make the Mixer connections.
6. Position the cursor over the right end of the **LTSLiq** stream icon.

   The connection point and pop-up Out appears.

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

7. With the pop-up visible, click and drag the cursor toward the left (inlet) side of the Mixer, and multiple connection points appear at the Mixer inlet.
8. Place the cursor near the inlet area of the Mixer.

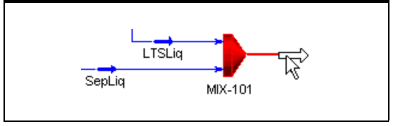
When the solid white box appears at the cursor tip, release the left mouse button to make the connection.

9. Repeat steps 5-8 to connect **SepLiq** to the Mixer.
10. Move the cursor over the right end of the Mixer icon.

    The connection point and pop-up Product appears.
11. With the pop-up visible, click and drag the cursor to the right of the Mixer.

    A white arrow stream icon appears.

Figure 1.81



12. With the stream icon visible, release the mouse button. UniSim Design will create a new stream with the default name **1**.
13. Release the **CTRL** key to leave Attach mode.
14. Double-click on the outlet stream icon **1** to access its property view.

    When you created the Mixer outlet stream, UniSim Design automatically combined the two inlet streams and flashed the mixture to determine the outlet conditions.

Close icon

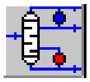
15. In the **Stream Name** cell, rename the stream to **TowerFeed**, then click the **Close** icon.

Installing the Column

UniSim Design 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.

In this section, you will install a Distillation Column.

1. From the **Tools** menu, select **Preferences**.
2. On the **Simulation** tab, **Options** page, ensure that the **Use Input Experts** checkbox is selected (checked), then close the view.
3. Press **F4** to access the Object Palette.

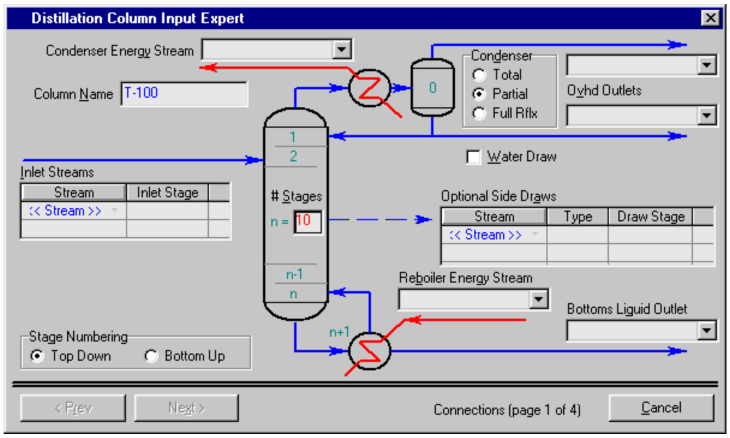


Distillation Column icon

4. Double-click on the **Distillation Column** icon on the Object Palette.

The first page of the Input Expert view appears.

Figure 1.82



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

When you install a column using a pre-built template, UniSim Design supplies certain default information, such as the number of stages. The current active cell is # Stages (Number of Stages), indicated by the thick border around this cell and the presence of 10 (default number of stages).

Some points worth noting:

- These are theoretical stages, as the UniSim Design default stage efficiency is one. If you want to specify real stages, you can change the efficiency of any or all stages later.
- The Condenser and Reboiler are considered separate from the other stages, and are not included in the Numb Stages field.

For this example, 10 theoretical stages will be used, so leave the Number of Stages at its default value.

5. Click on the **<<Stream>>** cell in the Inlet Streams table.
6. Open the drop-down list for the available feed streams by clicking the icon or pressing **F2** then the **DOWN** or **UP** arrow key.
7. Select **TowerFeed** as the inlet feed stream to the column.

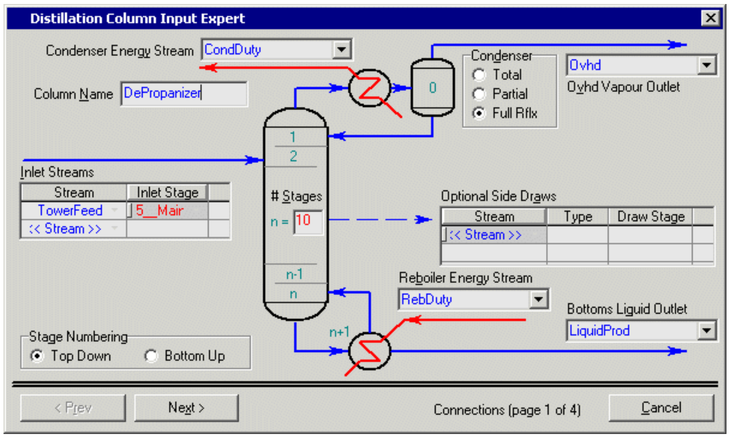
   UniSim Design will supply a default feed location in the middle of the Tray Section (TS), in this case stage 5 (indicated by 5_Main TS). This default location is used, so there is no need to change the Feed Stage.

   This column has Overhead Vapour and Bottoms Liquid products, but no Overhead Liquid (distillate) product.
8. In the Condenser group, select the **Full Rflx** radio button.

   The distillate stream disappears. This is the same as leaving the Condenser as Partial and later specifying a zero distillate rate.

9. Enter the stream and Column names as shown in the figure below.

Figure 1.83

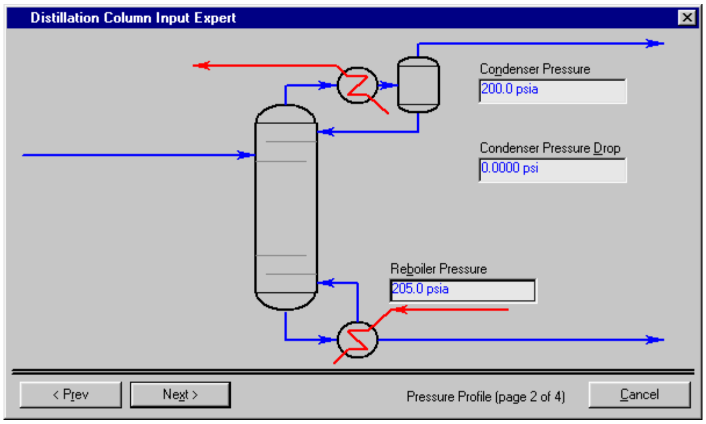


When you are finished, the **Next** button becomes active, indicating sufficient information has been supplied to advance to the next page of the Input Expert.

10. Click the **Next** button to advance to the **Pressure Profile** page.
11. In the **Condenser Pressure** field, enter **200 psia**.
12. In the **Reboiler Pressure** field, enter **205 psia**.

The Condenser Pressure Drop can be left at its default value of zero.

Figure 1.84

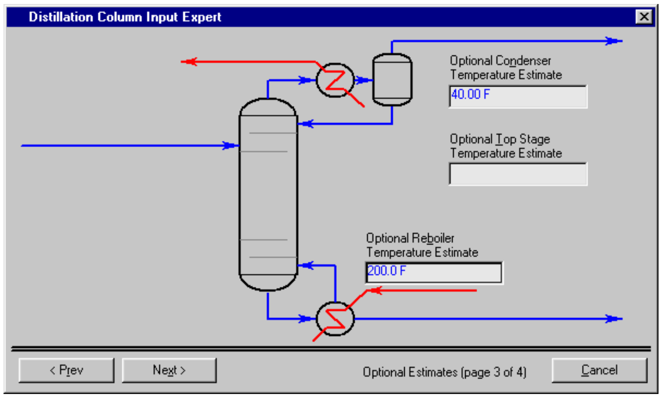


13. Click the **Next** button to advance to the **Optional Estimates** page.

Although UniSim Design does not require estimates to produce a converged column, good estimates will usually result in a faster solution.

14. Specify a **Condenser** temperature of **40°F** and a **Reboiler Temperature Estimates** of **200°F**.

Figure 1.85



15. Click the **Next** button to advance to the fourth and final page of the Input Expert.

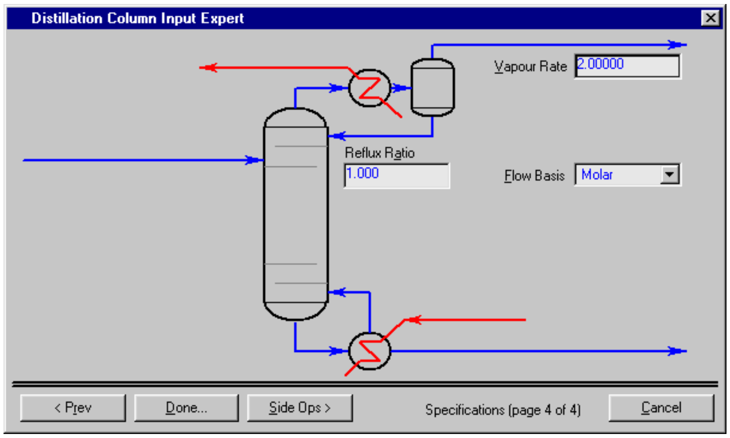
    The Specifications page allows you to supply values for the default column specifications that UniSim Design has created.

16. Enter a **Vapour Rate** of **2.0 MMSCFD** and a **Reflux Ratio** of **1.0**.

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

In general, a Distillation Column has three default specifications, however, by specifying zero overhead liquid flow (Full Reflux Condenser) one degree of freedom was eliminated. For the two remaining default specifications, overhead Vapour Rate is an estimate only, and Reflux Ratio is an active specification.

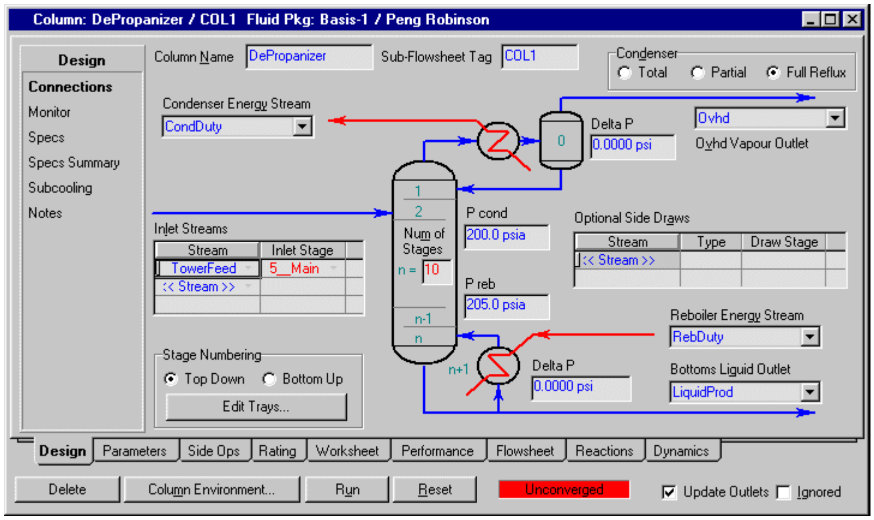
Figure 1.86



17. Click the **Done** button.

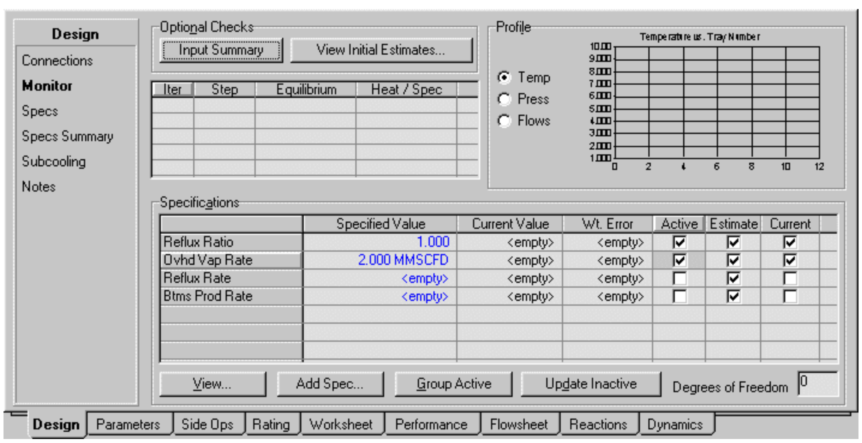
The Distillation Column property view appears.

Figure 1.87



18. Select the **Monitor** page.

Figure 1.88



The Monitor page displays the status of your column as it is being calculated, updating information with each iteration. You can also change specification values and activate or de-activate specifications used by the Column solver directly from this page.

Adding a Column Specification

The current Degrees of Freedom is zero, indicating the column is ready to be run. The Vapour Rate you specified in the Input Expert, however,

is currently an Active specification, and you want to use this only as an initial estimate for the solver for this exercise.

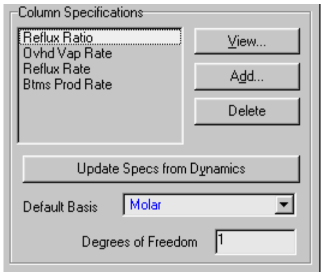
1. In the **Ovhd Vap Rate** row, click the **Active** checkbox to clear it, leaving the **Estimate** checkbox checked.

   The Degrees of Freedom will increase to 1, indicating that another active specification is required. For this example, a 2% propane mole fraction in the bottoms liquid will be specified.

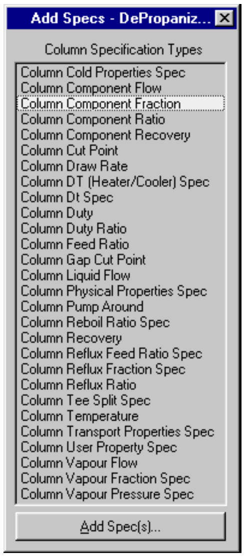
2. Select the **Specs** page.

   This page lists all the Active and non-Active specifications which are required to solve the column.

Figure 1.89



3. In the Column Specifications group, click the **Add** button. The Add Specs view appears.

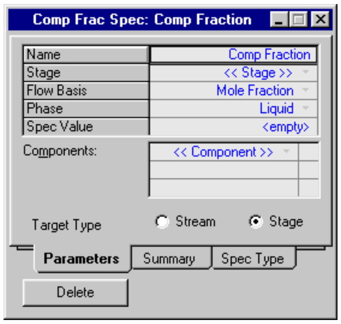


4. From the Column Specification Types list, select **Column Component Fraction**.

5. Click the **Add Spec(s)** button.

   The Comp Frac Spec view appears.

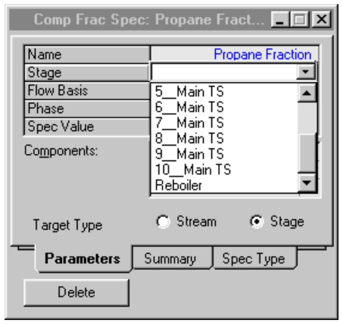
Figure 1.90



6. In the **Name** cell, change the specification name to **Propane Fraction**.

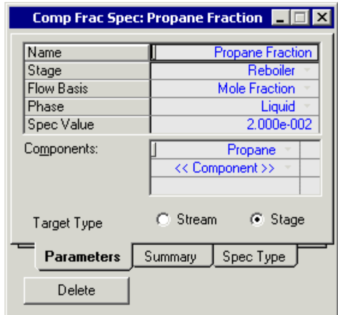
7. In the **Stage** cell, select **Reboiler** from the drop-down list of available stages.

Figure 1.91



8. In the **Spec Value** cell, enter **0.02** as the liquid mole fraction specification value.
9. Click in the first cell **<<Component>>** in the Components table, and select Propane from the drop-down list of available components.

Figure 1.92



10. Close this view to return to the Column property view.

    The new specification appears in the Column Specifications list on the **Specs** page.

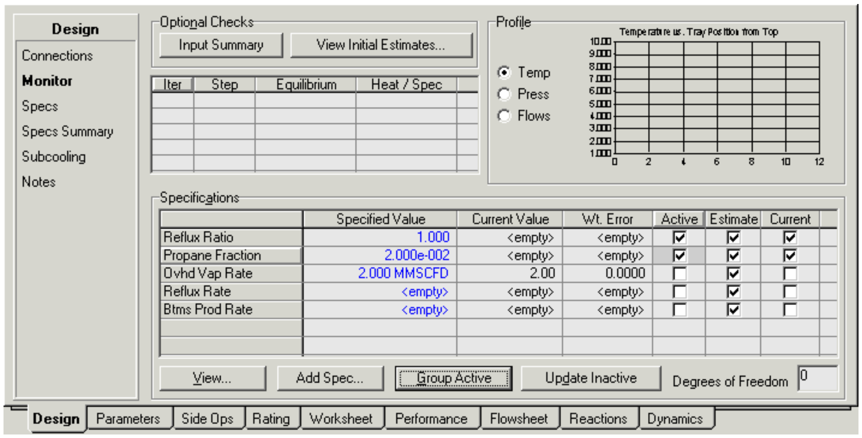
UniSim Design automatically made the new specification active when you created it.

11. Return to the **Monitor** page.

    The new specification may not be visible unless you scroll down the table because it has been placed 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 specification.

Figure 1.93



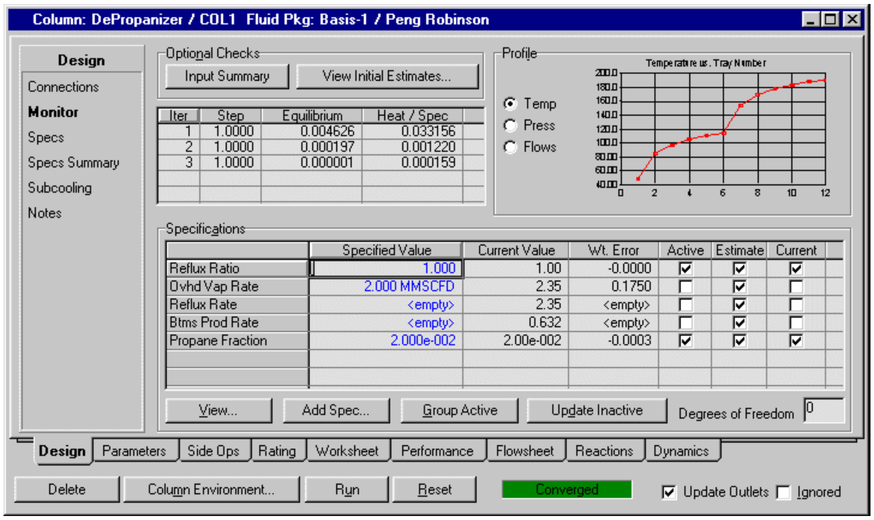
The Degrees of Freedom has returned to zero, so the column is ready to be calculated.

Running the Column

1. Click the **Run** button to begin calculations.

The information displayed on the **Monitor** page is updated with each iteration. The column converges quickly, in three iterations.

Figure 1.94



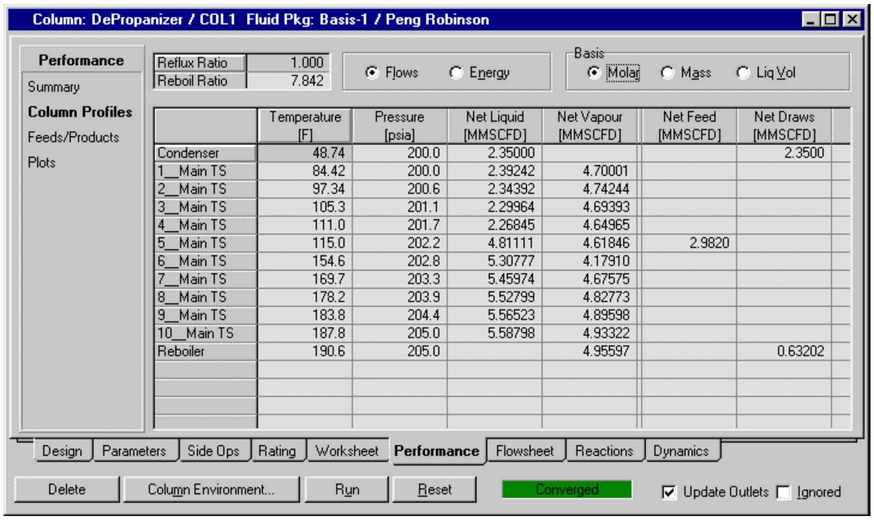
The table in the Optional Checks group displays the Iteration number, Step size, and Equilibrium error and Heat/Spec error.

The column temperature profile appears in the Profile group.You can view the pressure or flow profiles by selecting the appropriate radio button

The status indictor has changed from Unconverged to Converged.

2. Click the **Performance** tab, then select the **Column Profiles** page to access a more detailed stage summary.

Figure 1.95



Accessing the Column Sub-flowsheet

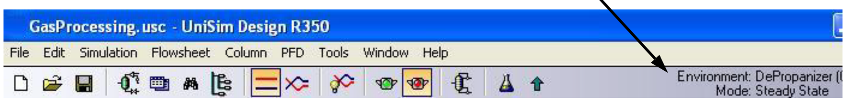
When considering the column, you might want to focus only on the column sub-flowsheet. You can do this by entering the column environment.

1. Click the **Column Environment** button at the bottom of the column property view.

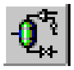
   UniSim Design desktop now displays the Column Sub-flowsheet environment.

Figure 1.96

The Environment label displays **DePropanizer (Col1)**.



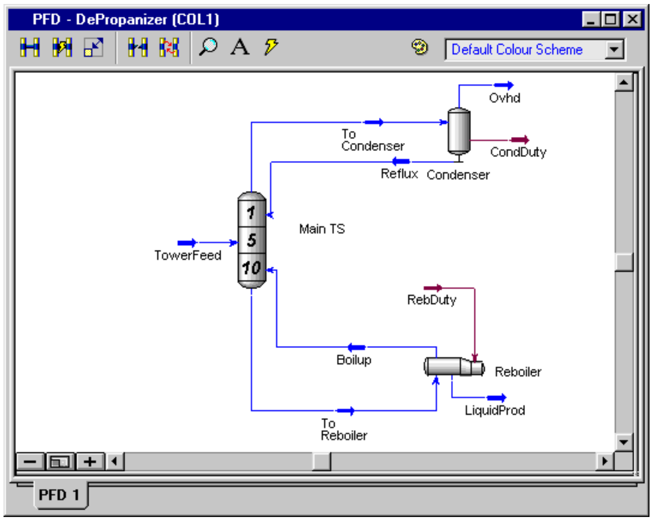
2. In this environment you can do the following:

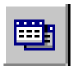


PFD icon

- Click the **PFD** icon to view the column sub-flowsheet PFD.

Figure 1.97

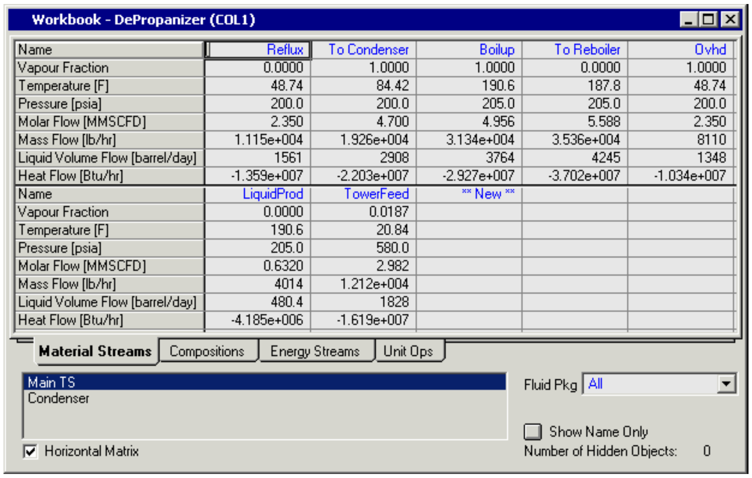




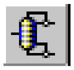
Workbook icon

- Click the **Workbook** icon to view a Workbook for the column sub-flowsheet objects.

Figure 1.98



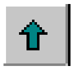
Name	Reflux	To Condenser	Boilup	To Reboiler	Ovhd
Vapour Fraction	0.0000	1.0000	1.0000	0.0000	1.0000
Temperature [F]	48.74	84.42	190.6	187.8	48.74
Pressure [psia]	200.0	200.0	205.0	205.0	200.0
Molar Flow [MMSCFD]	2.350	4.700	4.956	5.588	2.350
Mass Flow [lb/hr]	1.115e+004	1.926e+004	3.134e+004	3.536e+004	8110
Liquid Volume Flow [barrel/day]	1561	2908	3764	4245	1348
Heat Flow [Btu/hr]	-1.359e+007	-2.203e+007	-2.927e+007	-3.702e+007	-1.034e+007
Name	LiquidProd	TowerFeed	** New **		
Vapour Fraction	0.0000	0.0187			
Temperature [F]	190.6	20.84			
Pressure [psia]	205.0	580.0			
Molar Flow [MMSCFD]	0.6320	2.982			
Mass Flow [lb/hr]	4014	1.212e+004			
Liquid Volume Flow [barrel/day]	480.4	1828			
Heat Flow [Btu/hr]	-4.185e+006	-1.619e+007			



Column Runner icon

- Click the **Column Runner** icon to access the inside column property view.

  This property view is essentially the same as the outside, or main flowsheet, property view.



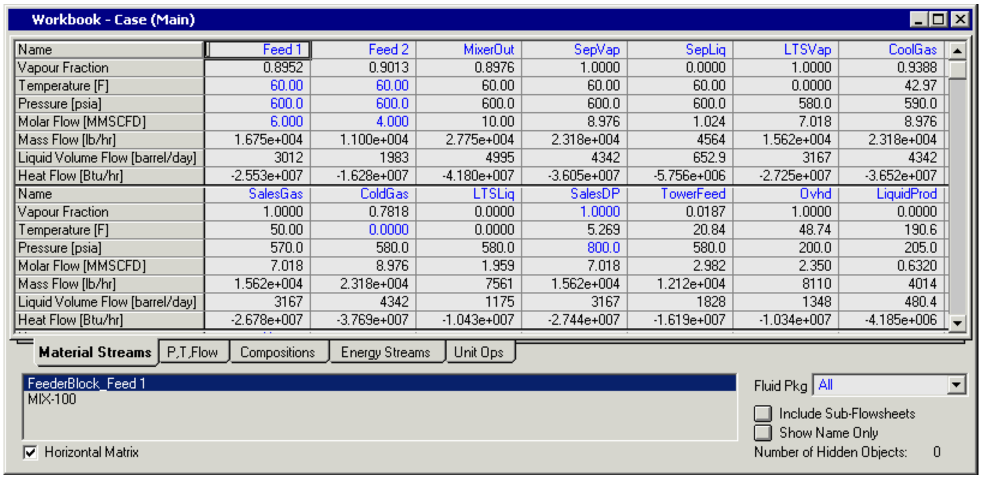
Enter Parent Simulation Environment icon

3. When you are finished in the column environment, return to the main flowsheet by clicking the **Enter Parent Simulation Environment** icon in the tool bar or the **Parent Environment** button on the column Worksheet view.

1.2.9 Viewing and Analyzing Results

1. Open the Workbook for the main case to access the calculated results for all streams and operations.
2. Click the **Material Streams** tab.

Figure 1.99



3. Click the **Compositions** tab.

Figure 1.100

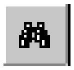
Name	Feed 1	Feed 2	MixerOut	SepVap	SepLiq	LTSVap	CoolGas
Comp Mole Frac (Nitrogen)	0.0100	0.0179	0.0132	0.0145	0.0017	0.0179	0.0145
Comp Mole Frac (CO2)	0.0100	0.0000	0.0060	0.0063	0.0034	0.0066	0.0063
Comp Mole Frac (Methane)	0.6000	0.6244	0.6098	0.6576	0.1905	0.7664	0.6576
Comp Mole Frac (Ethane)	0.2000	0.1666	0.1866	0.1846	0.2044	0.1565	0.1846
Comp Mole Frac (Propane)	0.1000	0.1136	0.1054	0.0877	0.2612	0.0414	0.0877
Comp Mole Frac (i-Butane)	0.0400	0.0431	0.0412	0.0272	0.1640	0.0070	0.0272
Comp Mole Frac (n-Butane)	0.0400	0.0345	0.0378	0.0222	0.1748	0.0043	0.0222
Name	SalesGas	ColdGas	LTSLiq	SalesDP	TowerFeed	Ovhd	LiquidProd
Comp Mole Frac (Nitrogen)	0.0179	0.0145	0.0021	0.0179	0.0020	0.0025	0.0000
Comp Mole Frac (CO2)	0.0066	0.0063	0.0053	0.0066	0.0046	0.0059	0.0000
Comp Mole Frac (Methane)	0.7664	0.6576	0.2677	0.7664	0.2412	0.3061	0.0000
Comp Mole Frac (Ethane)	0.1565	0.1846	0.2854	0.1565	0.2576	0.3269	0.0000
Comp Mole Frac (Propane)	0.0414	0.0877	0.2534	0.0414	0.2561	0.3196	0.0200
Comp Mole Frac (i-Butane)	0.0070	0.0272	0.0998	0.0070	0.1218	0.0339	0.4490
Comp Mole Frac (n-Butane)	0.0043	0.0222	0.0862	0.0043	0.1166	0.0052	0.5309

Using the Object Navigator

In this section, you will use the Object Navigator to view properties for a particular stream or operation. The Object Navigator allows you to quickly access the property view for any stream or unit operation at any time during the simulation.

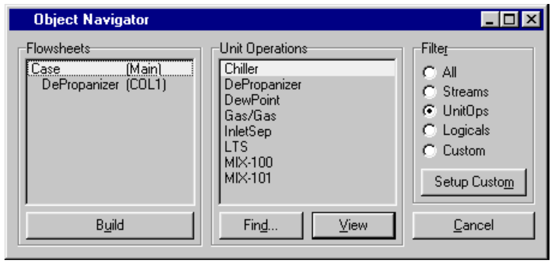
1. To open the Navigator, do **one** of the following:
   - Press **F3**.
   - From the **Flowsheet** menu, select **Find Object**.
   - Click the **Object Navigator** icon.

   The Object Navigator view appears:



Object Navigator icon

Figure 1.101



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

2. To open a property view, select the operation in the list and click the **View** button, or double-click on the operation.

- To change which objects appear, select a different radio button in the Filter group.
- To list all streams and unit operations, select the **All** button.

3. 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. UniSim Design opens the property view for the object.

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.

Using the Databook

The UniSim Design 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.

For this example, the effects of LTS temperature on the Sales Gas dew point and flow rate, and the Liquid Product flow rate will be examined.

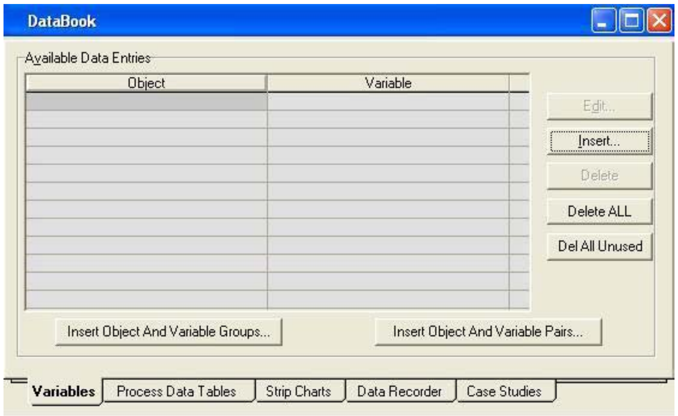
Defining the Key Variables

Before opening the Databook, close the Object Navigator or any property view you might have opened using the Navigator.

1. To open the Databook, do **one** of the following:
   - Press **CTRL D**.
   - Open the **Tools** menu and select **Databook**.

   The Databook appears as shown below.

Figure 1.102



2. Click the **Variables** tab.

   Here you will add the key variables to the Databook.

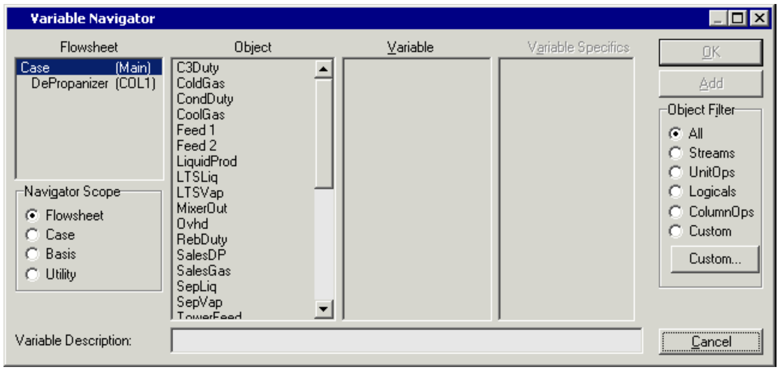
The Variable Navigator is used extensively in UniSim Design for locating and selecting variables.

The Navigator operates in a left-to-right manner. The selected Flowsheet determines the Object list; the chosen Object dictates the Variable list; the selected Variable determines whether any Variable Specifics are available.

3. Click the **Insert** button.

   The Variable Navigator view appears.

Figure 1.103

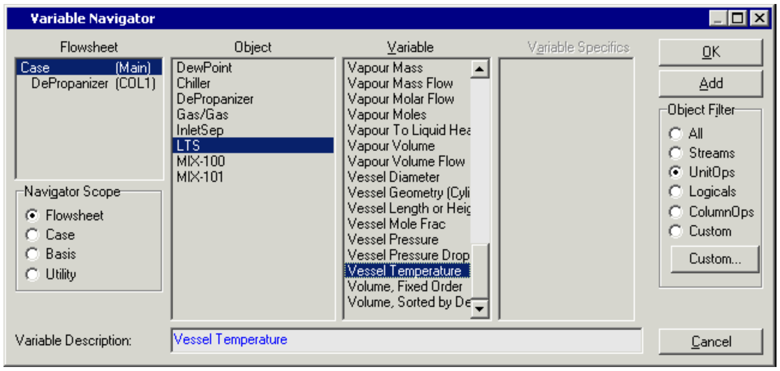


4. In the Object Filter group, select the **UnitOps** radio button. The Object list will be filtered to show unit operations only.
5. In the Object list, select **LTS**.

   The Variable list available for the LTS appears to the right of the Object list.
6. In the Variable list, select **Vessel Temperature**.

   UniSim Design displays this variable name in the **Variable Description** field.

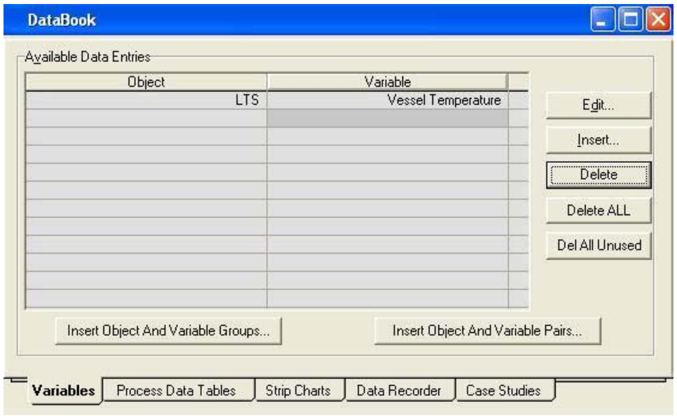
Figure 1.104



7. Click the **OK** button to add this variable to the Databook.

The new variable Vessel Temperature appears in the Databook.

Figure 1.105



Continue adding variables to the Databook.

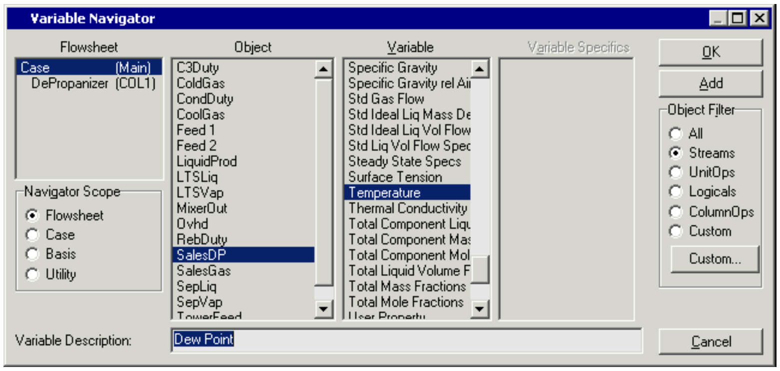
8. Click the **Insert** button, and the Variable Navigator reappears.
9. In the Object Filter group, select the **Streams** radio button. The Object list is filtered to show streams only.
10. In the Object list, select **SalesDP**.

The Variables list available for material streams appears to the right of the Object list.

11. In the Variable list, select **Temperature**.
12. In the **Variable Description** field, change description to **Dew Point**, then click the **Add** button.

    The variable now appears in the Databook, and the Variable Navigator view remains open.

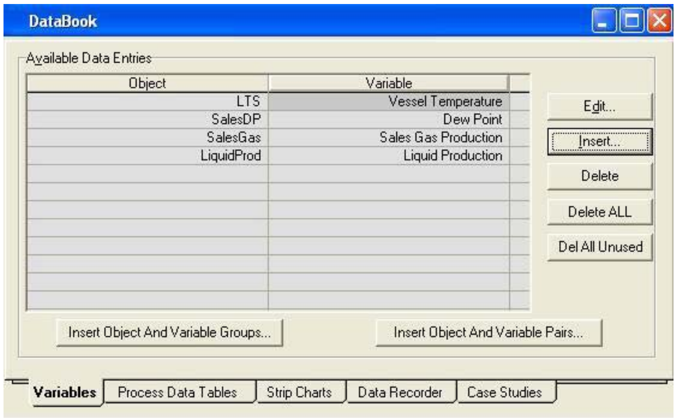
Figure 1.106



13. Repeat the previous steps to add the following variables to the Databook:
    - **SalesGas** stream; **Molar Flow** variable; change the Variable Description to **Sales Gas Production**
    - **LiquidProd** stream; **Liq Vol Flow@Std Cond** variable; change the Variable Description to **Liquid Production**
14. Click the **Close** button to close the Variable Navigator view.

    The completed Variables tab of the Databook appears as shown below.

Figure 1.107



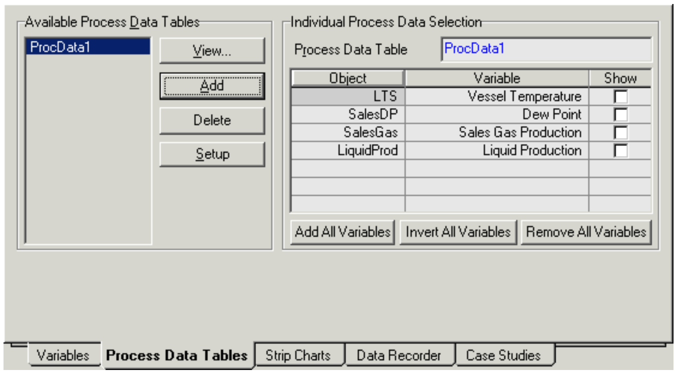
Creating the Data Table

In this section you will create a data table to display the variables.

1. Click the **Process Data Tables** tab.
2. In the Available Process Data Tables group, click the **Add** button.

   UniSim Design creates a new table with the default name ProcData1.

Figure 1.108



The four variables that were added to the Databook appear in the table on this tab.

3. In the **Process Data Table** field, change the name to **Key Variables**.
4. Activate each variable by clicking on the corresponding **Show** checkbox.

Figure 1.109

Object	Variable	Show
LTS	Vessel Temperature	☑
SalesDP	DewPoint	☑
SalesGas	Sales Gas Production	☑
LiquidProd	Liquid Production	☑

5. Click the **View** button to view the Key Variables Data table, which appears below.

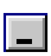
Figure 1.110

Key Variables Data

	Object	Variable	Value	Units	Tag	Access Mode
1	LTS	Vessel Temperature	0.0000	F	No Tag	No Transfer
2	SalesDP	Dew Point	5.269	F	No Tag	No Transfer
3	SalesGas	Sales Gas Production	7.018	MMSCFD	No Tag	No Transfer
4	LiquidProd	Liquid Production	479.7	barrel/day	No Tag	No Transfer

View DataBook...

You will access this table again later to demonstrate how its results are updated whenever a flowsheet change is made.



Minimize icon

6. For now, click the **Minimize** icon in the upper right corner of the Key Variables Data view.

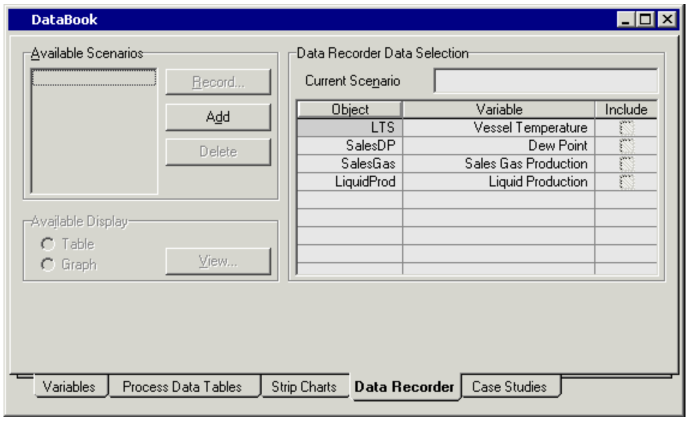
   UniSim Design reduces the view to an icon and places it at the bottom of the Desktop.

Using the Data Recorder

In this section you will use the Data Recorder to automatically record the current values of the key variables before making any changes to the flowsheet.

1. On the DataBook view, click the **Data Recorder** tab.

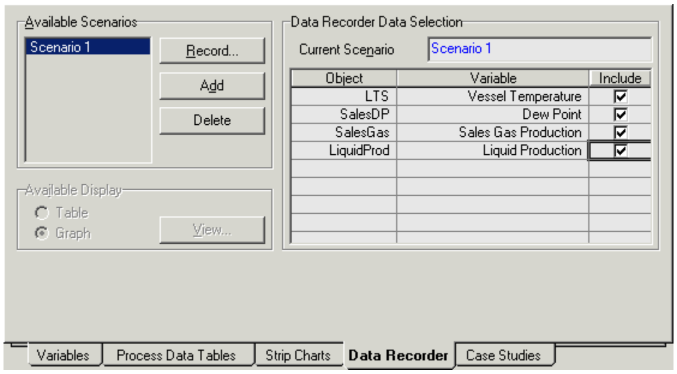
Figure 1.111



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

2. In the Available Scenarios group, click the **Add** button. UniSim Design creates a new scenario with the default name Scenario 1.
3. In the table, activate each variable by clicking on the corresponding **Include** checkbox.

Figure 1.112



4. 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.
5. Enter the new name **Base Case**, then click **OK**.

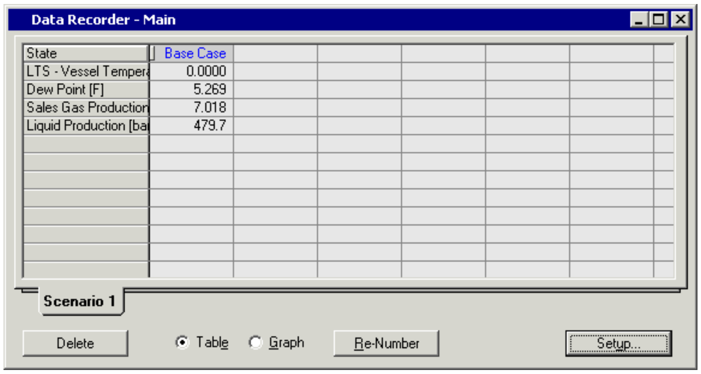
   The New Solved State view close and you return to the Databook

view.

6. In the Available Display group, select the **Table** radio button.
7. Click the **View** button.

   The Data Recorder appears, displaying the values of the key variables in their current state.

Figure 1.113



   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.

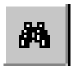
Minimize icon

Restore Up icon

8. Click the **Minimize** button to reduce the Data Recorder to an icon.
9. Click the **Restore Up** icon on the Key Variables Data view to restore the view to its original size.

Modifying the ColdGas Stream

In this section, you will change the temperature of stream ColdGas (which determines the LTS temperature) and view the changes in the process data table.

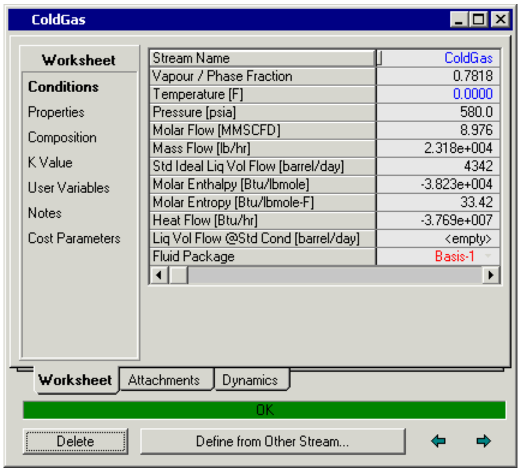


Object Navigator icon

1. Click the **Object Navigator** icon on the toolbar. The Object Navigator view appears
2. In the Filter group, select the **Streams** radio button.
3. In the Streams list, select **ColdGas**, then click the **View** button.

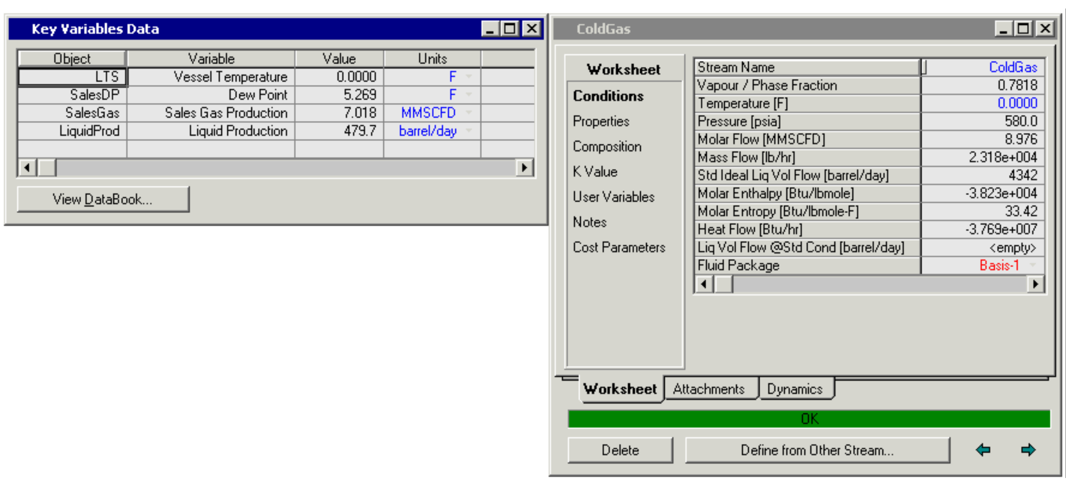
The ColdGas property view appears.

Figure 1.114



4. Ensure that you are on the **Worksheet** tab, **Conditions** page of the property view.
5. Arrange the two views, as shown below, by clicking and dragging on their title bars.

Figure 1.115



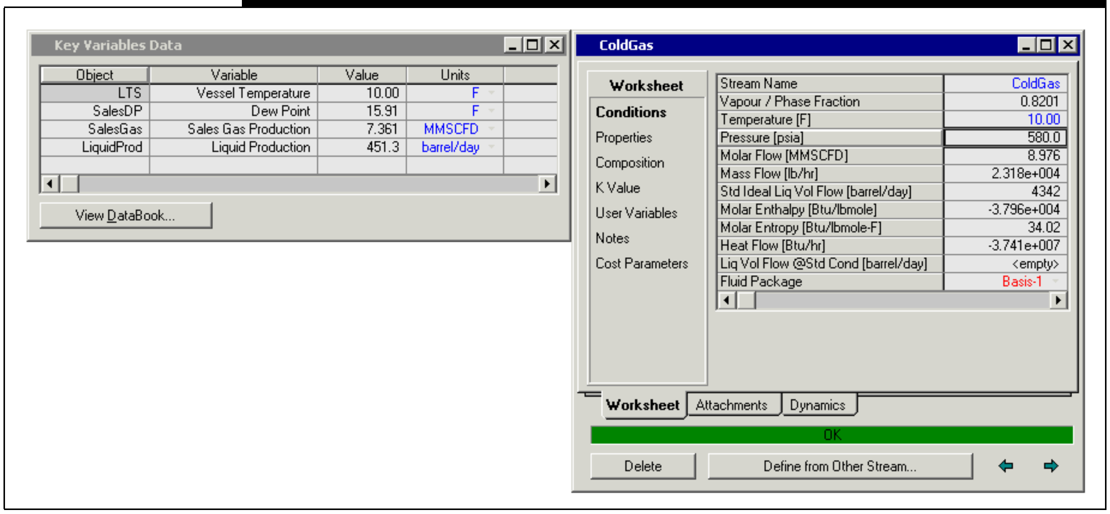
Currently, the LTS temperature is **0°F**. The key variables will be checked at **10°F**.

6. In the ColdGas **Temperature** cell, type **10°F**.

UniSim Design automatically recalculates the flowsheet. The new

results are shown below.

Figure 1.116



The change in Temperature generates the following results:

- The Sales Gas flow rate has increased.
- The Liquid Product flow rate has decreased.
- The sales gas dew point has increased to **15.9^{o}F**. This temperature no longer satisfies the dew point specification of **15^{o}F**.

Close icon

7. Click the **Close** icon on the ColdGas stream property view and return to the Databook.

Recording the New Variables in the Databook

In this section you will record the key variables in their new state.

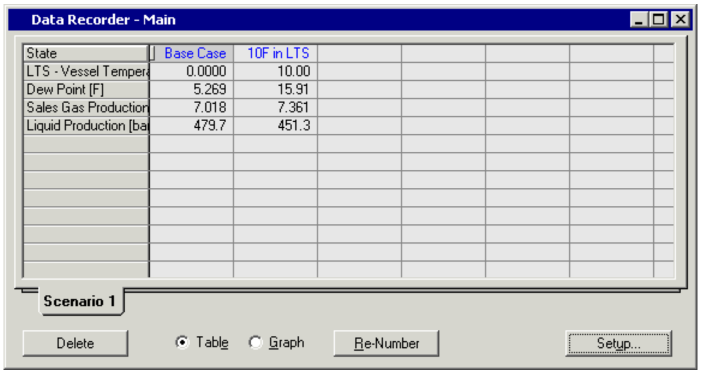
1. Click the **Data Recorder** tab in the Databook.
2. Click the **Record** button, and the New Solved State view appears.

   UniSim Design provides you with the default name State 2 for the new state.

3. Change the name to **10F in LTS**, then click the **OK** button to accept the new name.

4. Click the **View** button and the Data Recorder appears, displaying the new values of the variables.

Figure 1.117



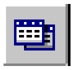
Close icon

5. Click the **Close** icon on the Data Recorder, then on the Databook, and finally on the Key Variables Table.
6. Save the case.

The basic simulation for this example has now been completed. You can continue with this example by proceeding to the Optional Study sections, or you can begin building your own simulation case. In the Optional Study, you will use some of the other tools available in UniSim Design to examine the process in more detail.

1.2.10 Optional Study

In the following sections, the effects of the LTS temperature on the SalesGas dew point and heating value are determined. Before proceeding, re-specify the temperature of ColdGas back to its original value of 0^{o}F:



Workbook icon

1. Click the Workbook icon on the toolbar.
2. On the **Material Streams** tab of the Workbook, click in the **Temperature** cell for the ColdGas stream.
3. Type **0**, then press **ENTER**.

Using the Spreadsheet

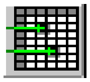
UniSim Design has a Spreadsheet operation that allows you to import stream or operation variables, perform calculations, and export calculated results.

Accessing the Spreadsheet

To install a Spreadsheet and display its property view:

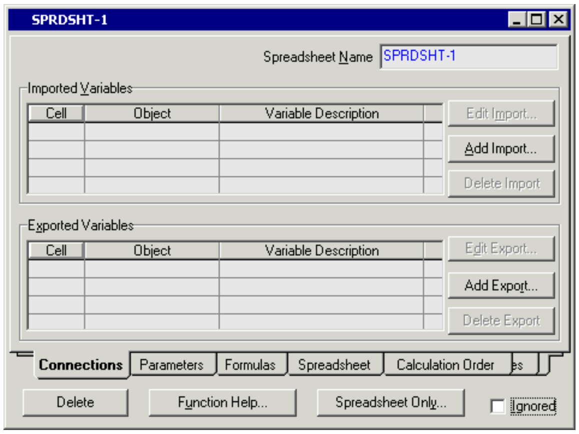
1. Access the Object Palette.
2. Double-click the **Spreadsheet** icon in the Object Palette.

   The Spreadsheet property view appears.



Spreadsheet icon

Figure 1.118



3. On the **Connections** tab, change the spreadsheet name to **Heating Value**.

   The heating value of the sales gas is calculated by importing the stream composition into the Spreadsheet then multiplying the mole fraction of each component by its individual heating value.

Importing Variables - First Method

In this section you will import variables on the Connections tab.

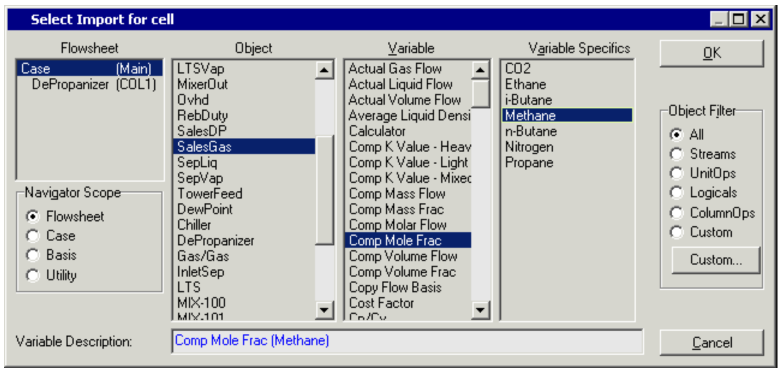
1. Click the **Add Import** button, and the Select Import for cell view

NO2 and CO2 are not included in the calculation as their individual heating values are negligible.

appears.

2. Choose the **SalesGas** Object, **Comp Mole Frac** Variable, and **Methane** Variable Specific as shown.

Figure 1.119

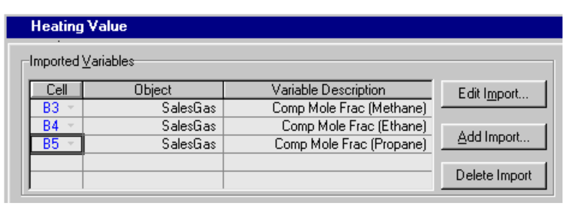


3. Click the **OK** button.
4. Click the **Add Import** button again, then select the **SalesGas** Object, **Comp Mole Frac** Variable, and **Ethane** Variable Specific.
5. Click the **OK** button.
6. Repeat steps 4 and 5 to add the **Propane** Variable Specific.

   For illustration purposes, the two remaining components will be added later using an alternative import method. UniSim Design assigned the imported variables to Spreadsheet cells A1 through A3, by default.

7. Change the cell locations to **B3** through **B5** as shown in the following figure; the reason for doing so will become apparent on the Spreadsheet tab.

Figure 1.120



8. No information is required on the Parameters and Formulas tabs, so click the **Spreadsheet** tab.
9. Enter the column headings as shown in the table below.

Column/Row	Heading
A1	Component
B1	Mole Fraction

Column/Row	Heading
C1	Comp Heat Value
D1	Total Heat Value

The UniSim Design Spreadsheet behaves similarly to commercial spreadsheet packages; you enter data and formulas in the cells, and calculated results are returned.

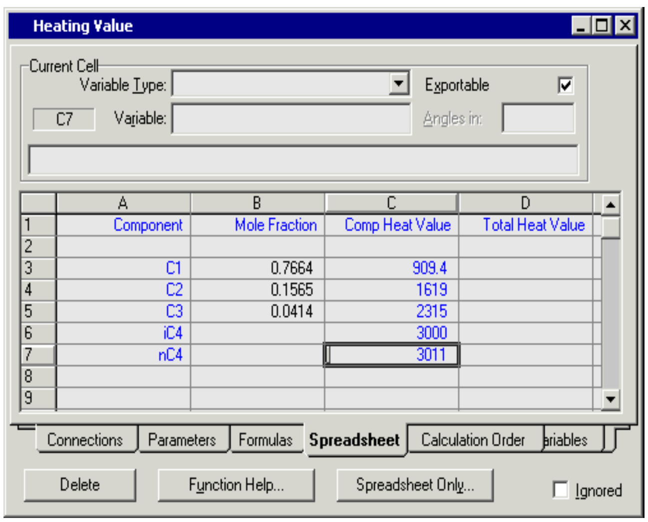
You can move to a cell by clicking it, or by pressing the arrow keys.

10. Enter the components in the Component column as shown as shown in the table below.

Row	Component
3	C1
4	C2
5	C3
6	iC4
7	nC4

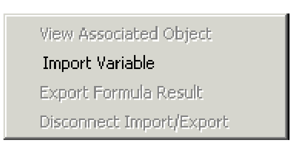
11. Enter the component net heating values in the Comp Heat Value column as shown in the figure below.

Figure 1.121



Importing Variables - Second Method

The next task is to import the remaining two variables' mole fractions in the Sales Gas.



Object Inspect menu

1. Select the Spreadsheet cell **B6**, which is reserved for the i-C4 mole fraction.
2. Right-click and select **Import Variable** from the Object Inspect menu.

   The Select Import for cell view appears.

3. Select the **SalesGas** Object, **Comp Mole Frac** Variable, and **i-Butane** Variable Specific.
4. Click the **OK** button to accept the input and close the view.
5. Follow steps 1 to 4 to import the mole fraction for **n-C4** into cell **B7**.
   - Position the cursor over cell **B7**.
   - Right-click once, and select **Import Variable**.
   - Select the **SalesGas** Object, **Comp Mole Frac** Variable, and **n-Butane** Variable Specific.
   - Click the **OK** button.

Entering Formulas

The next task is entering the formulas for calculating the component and total sales gas heating values.

All formulas must be preceded by a **=**.

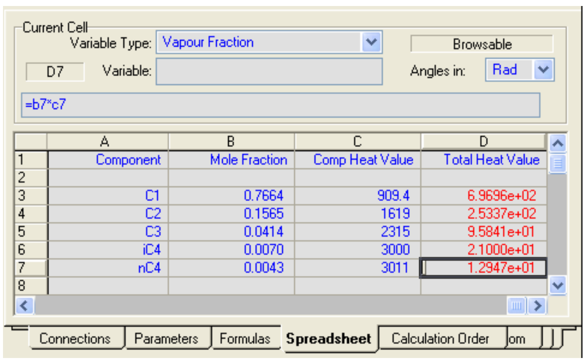
1. Click in cell **D3**.
2. Type **=b3*c3**, then press **ENTER**.

   This multiplies the Methane mole fraction by its Net Heating Value.
3. Enter the following formulas in cells **D4** through **D7**.

Cell	Formula
D4	=b4*c4
D5	=b5*c5
D6	=b6*c6
D7	=b7*c7

4. The table should appear as shown in the figure below.

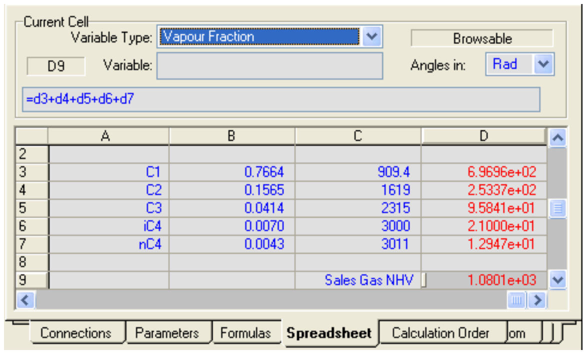
Figure 1.122



5. Click in cell **C9**, and type **Sales Gas NHV**.
6. Click in cell **D9**.
7. Enter **=d3+d4+d5+d6+d7** in cell **D9** to sum the individual heating values.

The result is the NHV of SalesGas in Btu/scf.

Figure 1.123



To add the value of Sales Gas NHV to the Databook:

1. Click the **Parameters** tab of the Heating Value property view.
2. In the Exportable Cells table, enter a Variable Name for cell **D9** (for example NHV).
3. Open the Databook by pressing **CTRL D**.
4. On the **Variables** tab, insert the variable, selecting the **Heating Value** operation as the Object and **NHV** as the variable.

The current heating value of the sales gas is **1080 Btu/scf**. Whenever flowsheet changes are made that result in the re-calculation of the stream SalesGas, the compositional changes will be automatically transferred to the Spreadsheet, and the heating value updated accordingly.

8. Close the Heating Value property view.

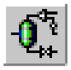
Installing an Adjust for Calculating the LTS Temperature

Suppose the market price of your liquid product is currently unfavourable and you want to raise the LTS temperature to leave more of the heavier components in the gas phase. This will increase the sales gas heating value, resulting in a bonus from the transmission company. The sales gas must, however, still comply with the dew point specification.

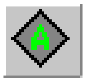
The Adjust operation performs automatic trial-and-error calculations until a target value is reached.

An Adjust operation can be used to adjust the temperature of the LTS (ColdGas stream) until the sales gas dew point is within a few degrees of the pipeline specification. In effect, this increases the gas heating value while still satisfying the dew point criteria.

Installing, Connecting, and Defining the Adjust

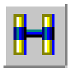


PFD icon



Adjust icon

1. Click the **PFD** icon to display the PFD and access the Object Palette by pressing **F4**.
2. Click the **Adjust** icon on the Object Palette.
3. Position the cursor on the PFD to the right of the **SalesDP** stream icon.



Attach Mode icon

4. Click to **drop** the Adjust icon onto the PFD.

   A new Adjust object appears with the default name **ADJ-1**.

5. Click the **Attach Mode** icon on the PFD toolbar to enter Attach mode.

6. Position the cursor over the left end of the **ADJ-1** icon.

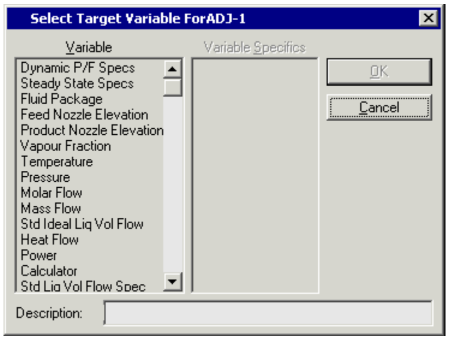
   The connection point and pop-up Adjusted Object appears.

7. With the pop-up visible, left-click and drag toward the **ColdGas** stream icon.

8. When the solid white box appears on the **ColdGas** stream, release the mouse button.

   The Select Adjusted Variable view appears.

Figure 1.124



At this point, UniSim Design knows that the ColdGas should be adjusted in some way to meet the required target. An adjustable variable for the ColdGas must now be selected from the Select Adjusted Variable view.

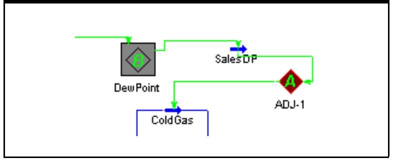
9. From the Variable list, select **Temperature**.
10. Click the **OK** button.
11. Position the cursor over the right corner of the **ADJ-1** icon. The connection point and pop-up Target Object appears.
12. With the pop-up visible, left-click and drag toward the **SalesDP** stream icon.
13. When the solid white box appears at the cursor tip, release the mouse button.

    The Select Target Variable view appears.

14. From the Variable list, select **Temperature**.

15. Click the **OK** button.

Figure 1.125



16. Click the **Attach Mode** icon to leave Attach mode.
17. Double-click the **ADJ-1** icon to open its property view.

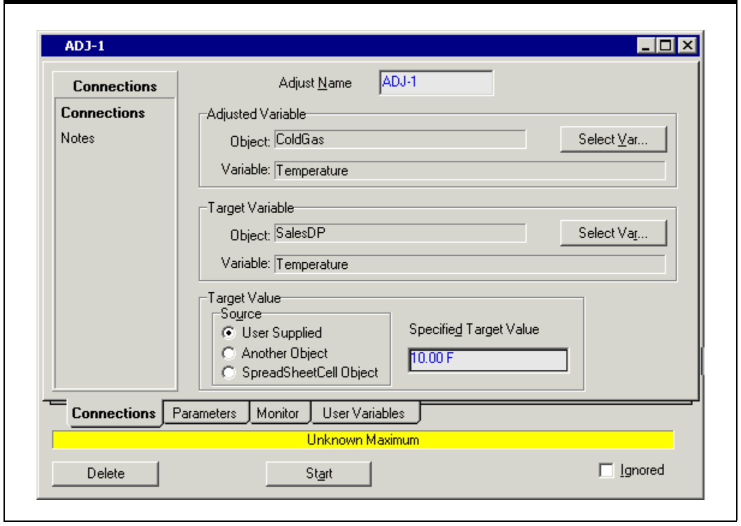
    The connections made in the PFD have been transferred to the appropriate cells in the property view.

Adjusting the Target Variable

The next task is to provide a value for the target variable, in this case the dew point temperature. A **5°F** safety margin will be used on the pipeline specification of **15°F**, so the desired dew point is **10°F**.

1. In the **Connections** page, enter **10°F** in the **Specified Target Value** field.

Figure 1.126

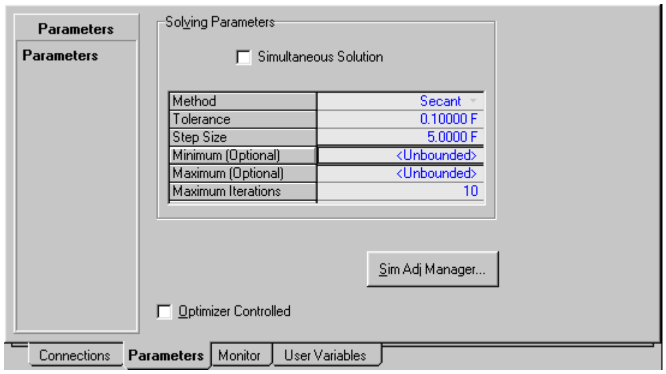


2. Click the **Parameters** tab.
3. In the **Parameters** page, enter **0.1°F** in the **Tolerance** cell.
4. In the **Step Size** cell, enter **5°F**.

    No values will be entered in the **Minimum** and **Maximum** field, as

these are optional parameters.

Figure 1.127



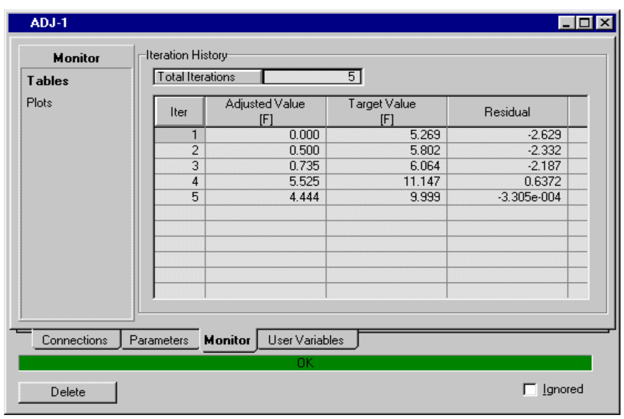
5. Click the **Monitor** tab.

   This tab enables you to view the calculations.

6. Click the **Start** button.

   The Adjust converges on the target value within the specified tolerance in five iterations. An LTS temperature (adjusted variable) of **4.4°F** gives a sales gas dew point (target variable) of 10°F.

Figure 1.128



The Adjust has changed the LTS temperature from the original value of **0°F** to **4.4°F**. The new sales gas heating value can now be compared to the previous value to see the effect of this change.

Close icon

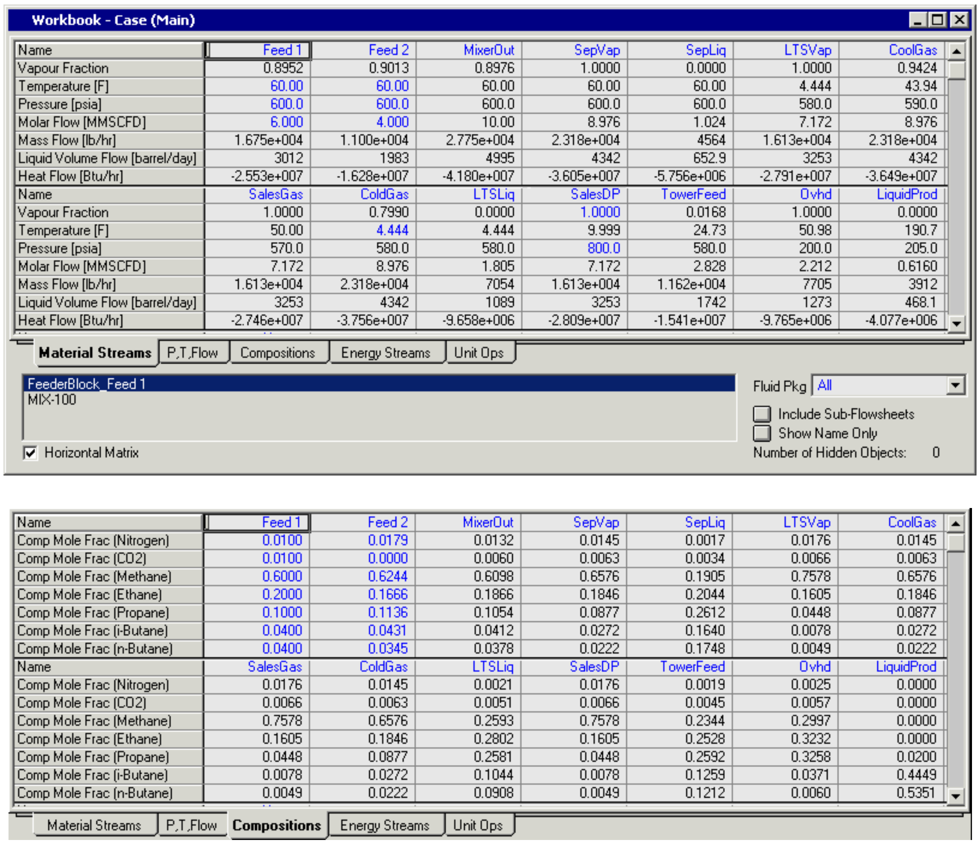
7. Click the **Close** icon on the Adjust property view.

Results of the Study

1. Open the Workbook to access the calculated results for the entire flowsheet.

   The Material Streams and Compositions tabs of the Workbook appear below.

Figure 1.129



Name	Feed 1	Feed 2	MixerOut	SepVap	SepLiq	LTSVap	CoolGas
Vapour Fraction	0.8952	0.9013	0.8976	1.0000	0.0000	1.0000	0.9424
Temperature [F]	60.00	60.00	60.00	60.00	60.00	4.444	43.94
Pressure [psia]	600.0	600.0	600.0	600.0	600.0	580.0	590.0
Molar Flow [MMSCFD]	6.000	4.000	10.00	8.976	1.024	7.172	8.976
Mass Flow [lb/hr]	1.675e+004	1.100e+004	2.775e+004	2.318e+004	4564	1.613e+004	2.318e+004
Liquid Volume Flow [barrel/day]	3012	1983	4995	4342	652.9	3253	4342
Heat Flow [Btu/hr]	-2.553e+007	-1.628e+007	-4.180e+007	-3.605e+007	-5.756e+006	-2.791e+007	-3.649e+007
Name	SalesGas	ColdGas	LTSLiq	SalesDP	TowerFeed	Ovhd	LiquidProd
Vapour Fraction	1.0000	0.7990	0.0000	1.0000	0.0168	1.0000	0.0000
Temperature [F]	50.00	4.444	4.444	9.999	24.73	50.98	190.7
Pressure [psia]	570.0	580.0	580.0	800.0	580.0	200.0	205.0
Molar Flow [MMSCFD]	7.172	8.976	1.805	7.172	2.828	2.212	0.6160
Mass Flow [lb/hr]	1.613e+004	2.318e+004	7054	1.613e+004	1.162e+004	7705	3912
Liquid Volume Flow [barrel/day]	3253	4342	1089	3253	1742	1273	468.1
Heat Flow [Btu/hr]	-2.746e+007	-3.756e+007	-9.658e+006	-2.809e+007	-1.541e+007	-9.765e+006	-4.077e+006

Name	Feed 1	Feed 2	MixerOut	SepVap	SepLiq	LTSVap	CoolGas
Comp Mole Frac (Nitrogen)	0.0100	0.0179	0.0132	0.0145	0.0017	0.0176	0.0145
Comp Mole Frac (CO2)	0.0100	0.0000	0.0060	0.0063	0.0034	0.0066	0.0063
Comp Mole Frac (Methane)	0.6000	0.6244	0.6098	0.6576	0.1905	0.7578	0.6576
Comp Mole Frac (Ethane)	0.2000	0.1666	0.1866	0.1846	0.2044	0.1605	0.1846
Comp Mole Frac (Propane)	0.1000	0.1136	0.1054	0.0877	0.2612	0.0448	0.0877
Comp Mole Frac (i-Butane)	0.0400	0.0431	0.0412	0.0272	0.1640	0.0078	0.0272
Comp Mole Frac (n-Butane)	0.0400	0.0345	0.0378	0.0222	0.1748	0.0049	0.0222
Name	SalesGas	ColdGas	LTSLiq	SalesDP	TowerFeed	Ovhd	LiquidProd
Comp Mole Frac (Nitrogen)	0.0176	0.0145	0.0021	0.0176	0.0019	0.0025	0.0000
Comp Mole Frac (CO2)	0.0066	0.0063	0.0051	0.0066	0.0045	0.0057	0.0000
Comp Mole Frac (Methane)	0.7578	0.6576	0.2593	0.7578	0.2344	0.2997	0.0000
Comp Mole Frac (Ethane)	0.1605	0.1846	0.2802	0.1605	0.2528	0.3232	0.0000
Comp Mole Frac (Propane)	0.0448	0.0877	0.2581	0.0448	0.2592	0.3258	0.0200
Comp Mole Frac (i-Butane)	0.0078	0.0272	0.1044	0.0078	0.1259	0.0371	0.4449
Comp Mole Frac (n-Butane)	0.0049	0.0222	0.0908	0.0049	0.1212	0.0060	0.5351

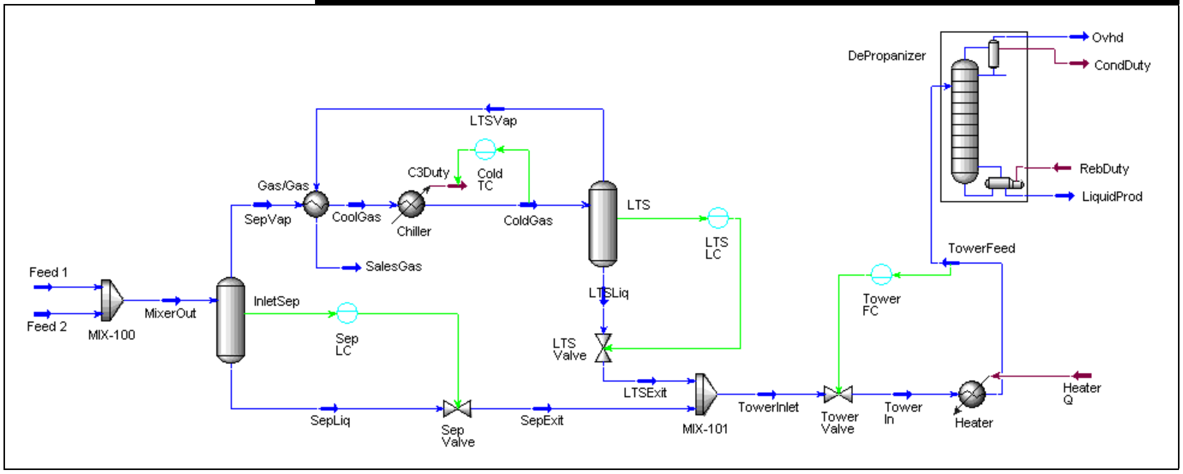
1.3 Dynamic Simulation

You can continue to this dynamic section with the case you built during the steady state section, or you can open the completed steady state version (which is the starting point for this dynamic section) called **TUTOR1.usc** in the UniSim Design\Samples directory.

In this tutorial, the dynamic capabilities of UniSim Design will be incorporated into a basic steady state gas plant model. The plant takes two different natural gas streams containing carbon dioxide and methane through n-butane and combines and processes them in a simple refrigeration system. A series of separators and coolers removes the heavier hydrocarbon components from the natural gas stream, allowing it to meet a pipeline dew point specification. The heavier liquid component of the gas stream is processed in a depropanizer column,

yielding a liquid product with a specified propane content.

Figure 1.130



This is only one method of preparing a steady state case for Dynamic mode.

The Dynamics Assistant will be used to make pressure-flow specifications and size pieces of equipment in the simulation flowsheet. It is also possible to set your own pressure-flow specifications and size the equipment without the aid of the Dynamics Assistant.

A completed dynamic case has been pre-built and is called **dyntut1.usc** in the UniSim Design\Samples directory.

This tutorial will comprehensively guide you through the steps required to add dynamic functionality to a steady state gas plant simulation.

To help you navigate these detailed procedures, the following milestones have been established for this tutorial:

1. Modify the steady state model so that a pressure-flow relation exists between each unit operation.
2. Implement a tray sizing utility for sizing the Depropanizer column.
3. Use the Dynamics Assistant to set pressure flow specifications and size the equipment in the simulation case.
4. Install and define the appropriate controllers.
5. Set up the Databook. Make changes to key variables in the process and observe the dynamic behaviour of the model.

In this Tutorial, you will follow this basic procedure in building the dynamic model.

1.3.1 Modifying the Steady State Flowsheet

It is necessary to add unit operations such as valves, heat exchangers, or pumps, to define pressure flow relations between unit operations that have no pressure flow relation. In this tutorial, valve operations will be added between Separator, Mixer, and Column operations.

A Heater operation will also be added between the Mixer and Column operation for dynamic simulation purposes. Installing a heater allows you to vary the temperature of the feed entering the column.

Valves will be added to the following material streams:

- SepLiq
- LTSLiq
- TowerFeed
- LiquidProd

The first task is to set the session preferences.

1. Open the pre-built case file **TUTOR1.usc**.

   The steady state Gas Processing simulation file TUTOR1.usc is located in your UniSim Design\Samples directory.

2. From the **Tools** menu, select **Preferences**.

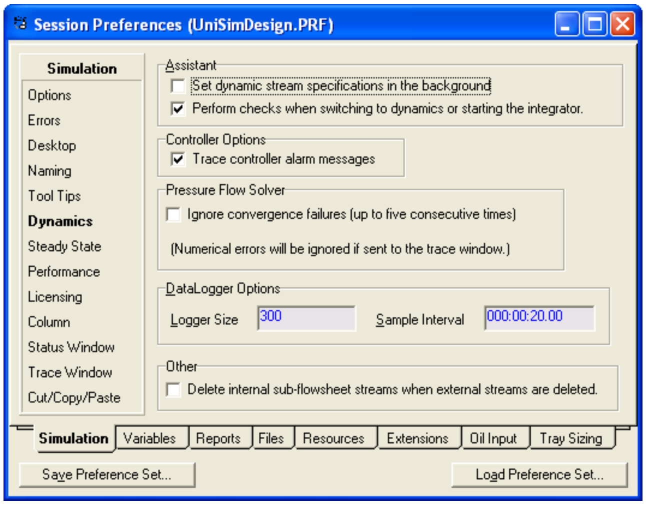
   The Session Preferences view appears.

3. Click the **Variables** tab, then select the **Units** page.

In the Dynamic simulation part of this tutorial you will work with the default Field units.

4. In the Available Unit Sets group list, select **Field**.
5. Click the **Simulation** tab, then select the **Dynamics** page.
6. In the Assistant group, uncheck both the **Set dynamic stream specifications in the background** and the **Perform checks when switching to dynamics or starting the integrator** checkboxes.

Figure 1.131



Close icon

7. Close the Session Preferences view along with all the open views on the UniSim Design desktop (except for the PFD view) by clicking the **Close** icon in the top right corner of each view.

   In the PFD, the stream pressure for Feed 2 will be deleted so that it

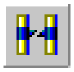
will be calculated by the MIX-100 in dynamic mode.

8. Double-click the **Feed 2** stream icon to open its property view.
9. On the **Conditions** page of the **Worksheet** tab, click in the **Pressure** cell, then press **DELETE** to remove the stream pressure.
10. Close the stream property view.

    Next you will change the pressure setting for the MIX-100 so that the whole PFD can be simulated.

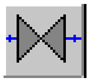
11. Double-click the **MIX-100** icon to open its property view.
12. On the **Design** tab, select the **Parameters** page.
13. In the Automatic Pressure Assignment group, click the **Equalize All** radio button.
14. Close the MIX-100 property view.

    Next you will insert a valve operation between the SepLiq stream and the MIX-101 unit operation.



Break Connection icon

15. Click the **Break Connection** icon in the PFD toolbar.
16. Break the SepLiq stream connection by doing the following:
    - Position the mouse pointer over the connection line between the SepLiq stream icon and the MIX-101 icon.
    - When the mouse pointer has a checkmark beside it, left-click and the SepLiq stream will disconnect from the MIX-101.
17. Open the Object Palette by pressing **F4**.



Valve icon

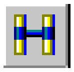
18. On the Object Palette, right-click and hold on the **Valve** icon.
19. Drag the cursor over the PFD.

    The mouse pointer becomes a bullseye.

20. Position the bullseye pointer beside the SepLiq stream and release the mouse button.
21. A Valve icon named VLV-100 appears.
22. Double-click the VLV-100 icon on the PFD to open its property view.
23. In the valve property view, specify the following connections:

Tab [Page]	In this cell...	Enter...
Design [Connections]	Name	Sep Valve
	Inlet	SepLiq
	Outlet	SepExit
Design [Parameters]	Delta P	25 psi

24. Click the **Close** icon to close the valve property view.
25. Connect the SepExit stream to the inlet of the MIX-101 unit operation by doing the following:
    - Click the PFD **Attach Mode** icon.
    - Position the mouse pointer at the tip of the SepExit stream arrow. A white box appears.



Attach Mode icon

- Click and drag the pointer to the left side of MIX-101. A white box appears, indicating a connection point.
- Release the mouse button to complete the connection.
- Click the **Attach Mode** icon again to exit from the attach mode.

Next you will insert a valve operation between the LTSLiq stream and the MIX-101 unit operation.

26. Break the line between the LTSLiq stream and the MIX-101 unit operation.
    - Click the **Break Connection** icon in the tool bar.
    - Click to the right of the arrow on the LTSLiq stream.
27. Install a second valve operation.
    - On the Object Palette, right-click the **Valve** icon.
    - Drag the cursor to the right of the LTSLiq stream.
    - Release the mouse button.
28. Double-click the valve icon to open its property view.
29. Specify the following connections:

Tab [Page]	In this cell...	Enter...
Design [Connections]	Name	LTS Valve
	Inlet	LTSLiq
	Outlet	LTSExit
Design [Parameters]	Delta P	5 psi

30. Close the valve property view.
31. Attach the LTSExit stream to the MIX-101 unit operation.
    - Click the **Attach Mode** icon
    - Move the cursor over the LTSExit stream icon. A white box appears.
    - Click and drag the cursor to the inlet side of the MIX-101 icon. A white box appears, indicating a connection point.
    - Release the mouse button to complete the connection.
    - Click the **Attach Mode** icon again to exit the attach mode.

    Next you will add a valve operation between the MIX-101 unit operation and the TowerFeed stream.
32. Break the line between the TowerFeed stream and the MIX-101 unit operation. Be sure to break the line to the left of the TowerFeed stream arrow.
33. Install a third valve operation with the following connections:

Tab [Page]	In this cell...	Enter...
Design [Connections]	Name	Tower Valve
	Inlet	TowerIn
	Outlet	TowerInlet
Design [Parameters]	Delta P	363 psi

You can use the scroll bars to navigate around the PFD.

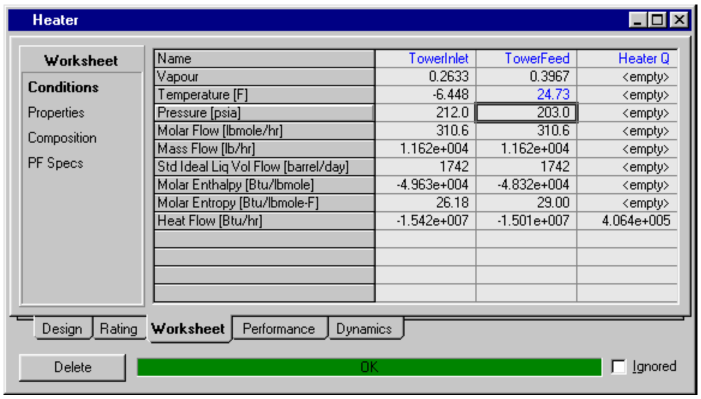
You can also use the **PAGE UP** and **PAGE DOWN** keys to zoom in and out of the PFD, respectively.

34. Close the valve property view.
35. Click the **Attach Mode** icon, then connect the TowerIn stream to the exit of the MIX-101 unit operation.
36. Exit the attach mode.
37. Install a Heater operation and position it near the Tower Valve and the DePropanizer.
    - In the Object Palette, click once on the **Heater** icon.
    - In the PFD, click where you want to insert the heater.
38. Open the heater property view and specify the following connections:

Tab [Page]	In this cell...	Enter...
Design [Connections]	Name	Heater
	Inlet	TowerInlet
	Outlet	TowerFeed
	Energy	Heater Q
Design [Parameters]	Delta P	9 psi

39. In the heater property view, click the **Worksheet** tab, then select the **Conditions** page.
40. In the **Temperature** cell of the TowerFeed stream, enter **24.73°F**.

Figure 1.132



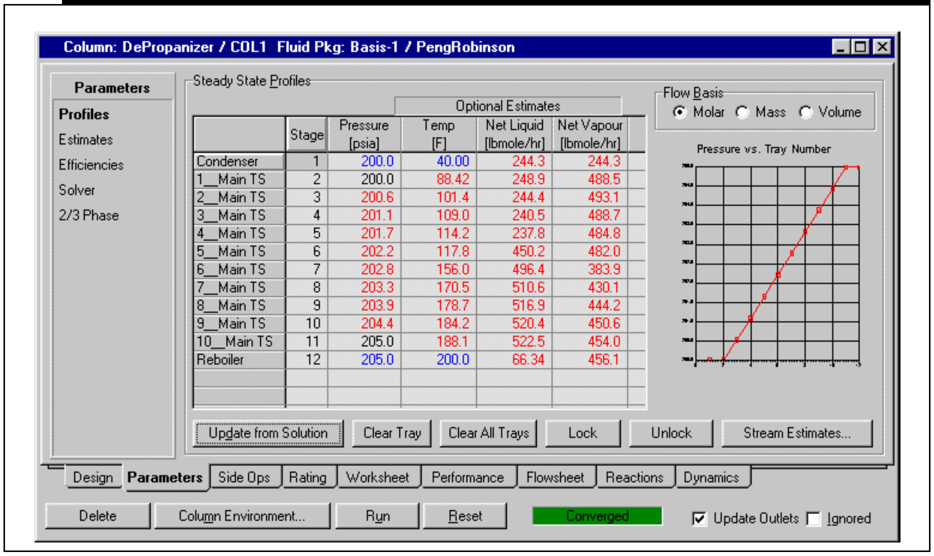
41. Close the Heater property view.

When considering pieces of equipment associated with a column, it may be necessary to enter the Column sub-flowsheet environment.

Next you will add a valve to the LiquidProd stream in the Column sub-flowsheet.

42. Double-click the DePropanizer column to open its property view.

Figure 1.133



43. Click the **Column Environment** button to enter the Column Sub-flowsheet environment.

    Next you will inset a valve operation between the LiquidProd stream and the Reboiler unit operation.

44. In the PFD of the column sub-flowsheet, break the connection between the **LiquidProd** stream and the **Reboiler** unit operation.

The Object Palette in the Column Environment contains fewer available unit operations than the Object Palette in the Parent Environment.

45. Press **F4** to open the Object Palette.

46. Install a valve operation between the Reboiler and the LiquidProd stream icon. Move the LiquidProd stream to make room if required.

47. Open the valve property view and specify the following connections:

Tab [Page]	In this cell...	Enter...
Design [Connections]	Name	Reboil Valve
	Inlet	LiquidExit
	Outlet	LiquidProd
Design [Parameters]	Delta P	25 psi

48. Close the valve property view.

49. Press **CTRL** to connect the **LiquidExit** stream to the liquid exit connection point of the **Reboiler**.

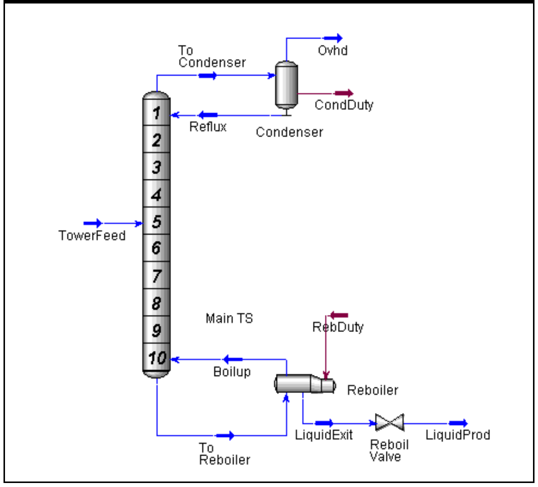
Run Column Solver icon

50. Click the **Run Column Solver** icon in the tool bar.

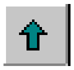
    The column will solve with the existing column specifications and

the added valve unit operations.

Figure 1.134



Next you will delete unit operations that have no impact on the Dynamic solver.



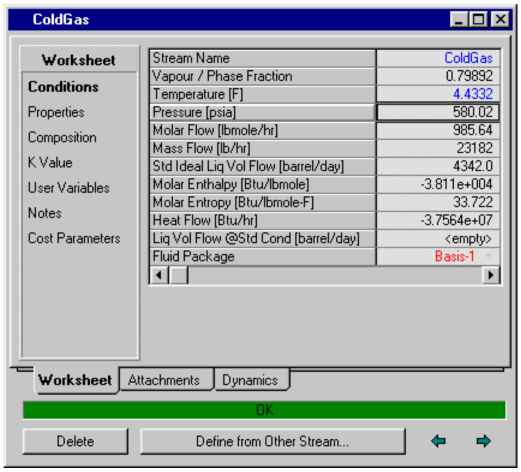
Enter Parent Simulation Environment icon

51. Return to the Main Flowsheet environment by clicking the **Enter Parent Simulation Environment** icon in the toolbar.
52. Close the DePropanizer column property view.

    The ADJ-1 and DewPoint logical operations have calculated the ColdGas stream temperature required to achieve a **10°F** dewpoint in the SalesGas stream.

53. In the PFD, double-click the **ColdGas** icon to open the stream property view.

Figure 1.135



54. Record the temperature of the ColdGas material stream so that it may be controlled in Dynamic mode:

Variable	Value
Cold Gas Stream Temperature	4.433°F

55. Close the ColdGas property view.

When you delete a stream, unit or logical operation from the flowsheet, UniSim Design will ask you to confirm the deletion.

56. On the PFD, click on the ADJ-1 logical operation icon, then press the **DELETE** key.
57. UniSim Design prompts you to confirm that you want to delete the object. Click the **Yes** button.
58. Delete the **DewPoint** logical operation and the **SalesDP** material stream from the PFD.

For more information on Session Preferences refer to **Section 12.5 - Files Tab** in the **UniSim Design User Guide**.

59. Ensure that the **Standard Windows file picker** radio button is selected on the **File** tab in the Session Preferences view.
60. From the **File** menu, select **Save As**. Save the file as **DynTUT1-1.usc**.

1.3.2 Column Sizing

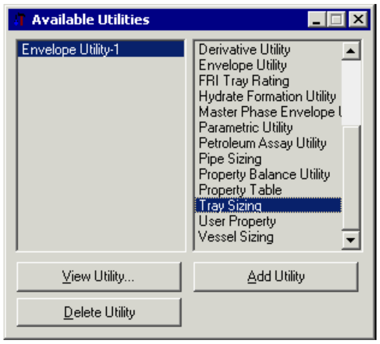
In preparation for Dynamic operation, the column and surrounding equipment must be sized. In the steady state environment, column pressure drop is user-specified. In dynamics, it is calculated using dynamic hydraulic calculations. Complications will arise in the transition from steady state to dynamics if the steady state pressure profile across the column is very different from that calculated by the dynamics pressure-flow solver.

Column Tray Sizing

1. To access the Available Utilities property view, do **one** of the following:
   - Press **CTRL U**.
   - From the **Tools** menu, select **Utilities**.

2. Scroll down the list of available utilities and select the **Tray Sizing** utility.

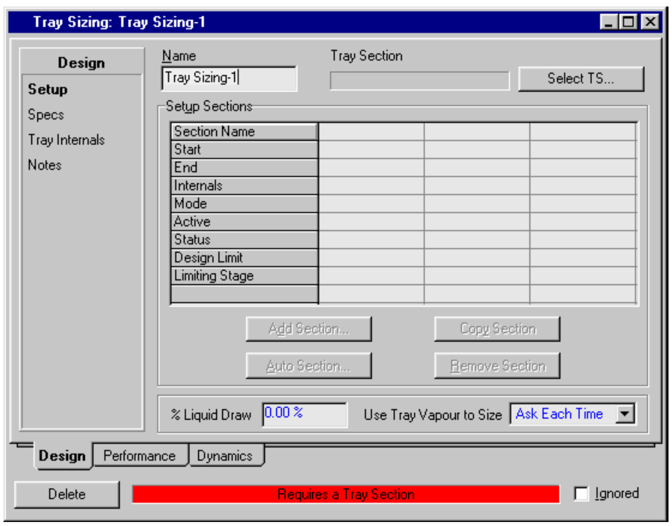
Figure 1.136



3. Click the **Add Utility** button.

   The Tray Sizing view appears.

Figure 1.137

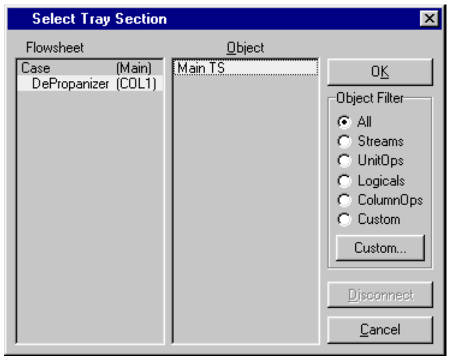


4. In the **Name** field, change the name to **DEPROP TS**.
5. Click the **Select TS** button.

   The Select Tray Section view appears.

6. In the Flowsheet group, select **DePropanizer**. In the Object group, select **Main TS**. Click the **OK** button.

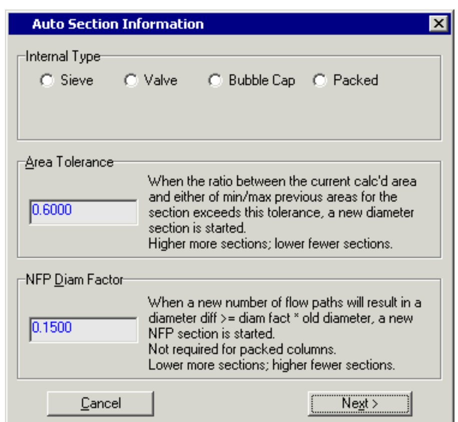
Figure 1.138



7. In the Setup Sections group, click the **Auto Section** button.

   The Auto Section Information view appears. The default tray internal types appear as follows:

Figure 1.139

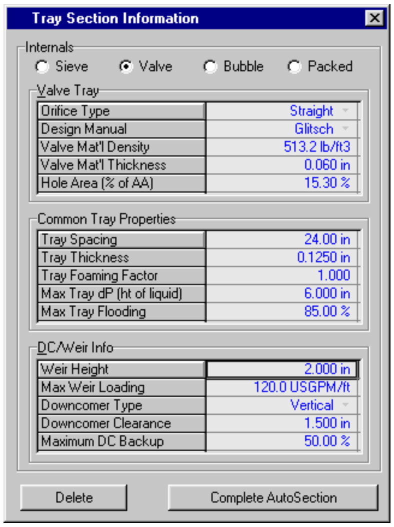


8. Select the **Valve** radio button and click **Next**.

   The Tray Section Information view displays the specific dimensions

of the valve-type trays.

Figure 1.140



9. Keep the default values. Click the **Complete AutoSection** button.

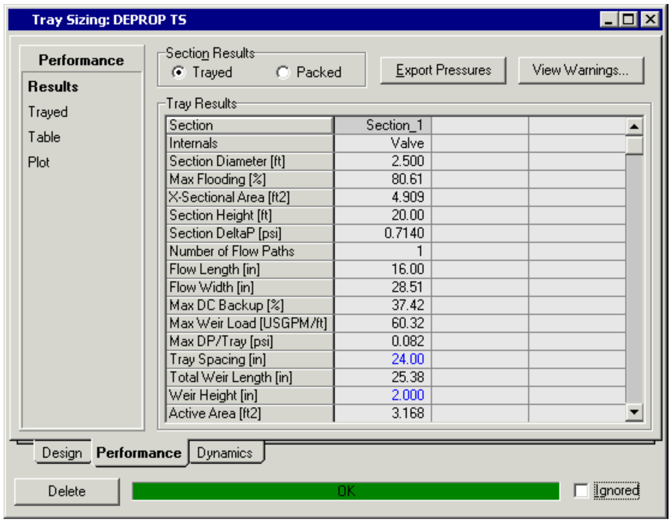
   UniSim Design calculates the Main TS tray sizing parameters based on the steady state flow conditions of the column and the desired tray types. UniSim Design labels the DePropanizer tray section as Section_1.

10. To confirm the dimensions and configuration of the trays for Section_1, click the **Performance** tab, then select the **Results** page.

    Confirm the following tray section parameters for Section_1, which

will be used for the Main TS tray sections.

Figure 1.141



Variable	Value
Section Diameter	2.5 ft
Weir Height	2 in
Tray Spacing	24 in
Total Weir Length	25.38 in

Remember the Max DP/Tray value on this page.

You can view column profile information on the Table and Plot pages.

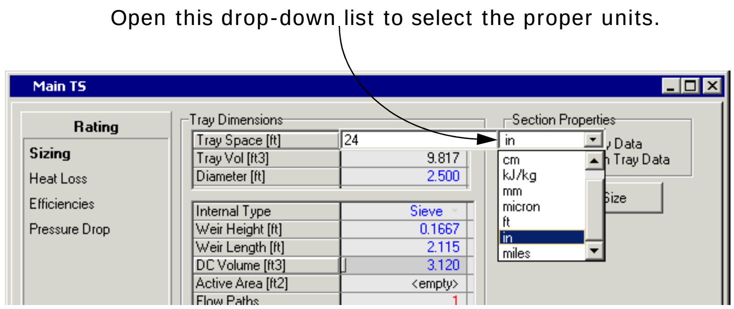
11. Click **Design** tab, then select the **Setup** page.
12. Select the **Active** checkbox.
13. On the **Results** page of the **Performance** tab, click the **Export Pressures** button. For now, ignore any warnings by clicking the **OK** button.
14. Close the Tray Sizing property view and the Available Utilities view.
15. Double-click the DePropanizer icon to open the Column property view.
16. Click the **Column Environment** button to enter the Column sub-flowsheet.
17. In the column PFD, double-click the Main TS Column object to open the Main TS property view.
18. Click the **Rating** tab, then select the **Sizing** page.
19. Enter the tray section parameters as follows:

Variable	Value
Diameter	2.5 ft
Weir Height	2 in

Variable	Value
Tray Space	24 in
Weir Length	25.38 in

Be aware that the units for each tray section parameter may not be consistent with the units appearing in the tray sizing utility. Use the drop-down list to select the units you want to input. UniSim Design automatically converts the value to the default unit.

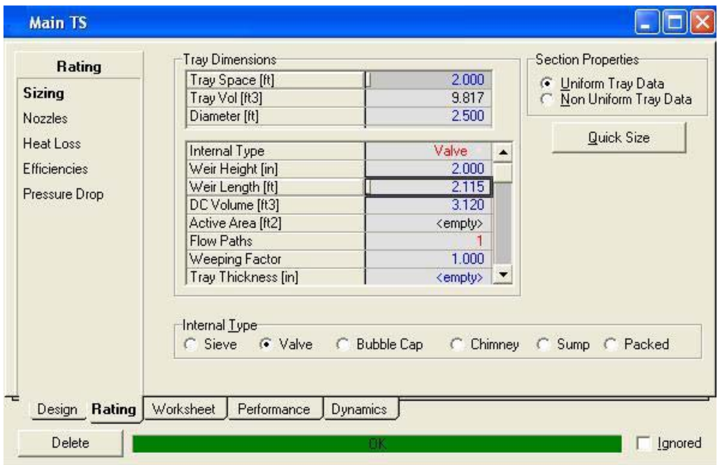
Figure 1.142



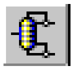
20. In the Internal Type group, select the **Valve** radio button.

    The complete Main TS tray section property view appears below:

Figure 1.143



21. Close the Main TS property view.



Column Runner icon

22. Access the Column property view by clicking the **Column Runner** icon.
23. In the **Profiles** page of the **Parameters** tab, note the steady state pressure profile across the column.

The theoretical top and bottom stage pressure should be calculated so that the pressure on stage 5_Main TS (the Tower Feed stage) is about **203 psia**, while the total pressure drop across the column is about **0.7 psi**.

24. In the Profiles group, Pressure column, click in the **Pressure** cell for the Condenser and press **DELETE**.
25. Click in the **Reboiler** pressure cell and press **DELETE**.
26. Click in the **Pressure** cell for the top stage (1_Main TS**)** and input a value of **202.6 psia**.
27. Specify the bottom stage pressure (10_Main TS) as **203.3 psia**.
28. Click the **Run** button at the bottom of the column property view to start the Column Solver.
29. Return to the Parent (Main) Simulation environment.
30. Save the case as **DynTUT1-2.usc**.

1.3.3 Using the Dynamics Assistant

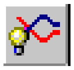
Before you can run the simulation case in Dynamic mode, the degrees of freedom for the flowsheet must be reduced to zero by setting the pressure-flow specifications. It is also necessary to size the existing valves, vessels, coolers, and heat exchangers in the Main Flowsheet and the Column Sub-flowsheet. The following sizing parameters must be specified for these unit operations:

Unit Operation	Sizing Parameter
Valves	Cv value
Vessels	Volume
Coolers/Heat Exchangers	k-values

The Dynamics Assistant makes recommendations as to how the flowsheet topology should change and what pressure-flow specifications are required in order to run a case in Dynamic mode. In addition, it automatically sets the sizing parameters of the equipment in the simulation flowsheet. Not all the suggestions that the Dynamics Assistant offers need to be followed.

The Dynamics Assistant will be used to do the following:

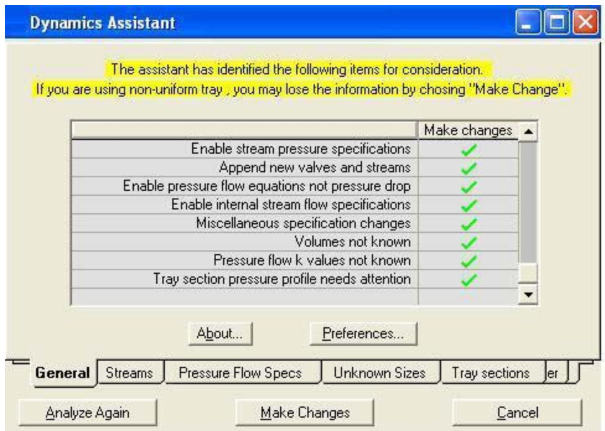
- Add Pressure-Flow specifications to the simulation case.
- Size the Valve, Vessel, and Heat Exchanger operations.



Dynamics Assistant icon

1. Click the **Dynamics Assistant** icon in the toolbar.

Figure 1.144



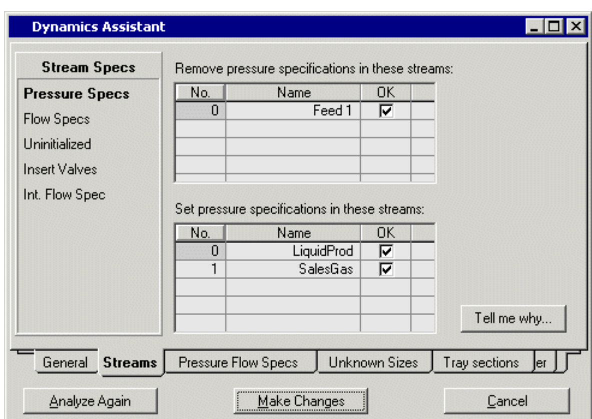
Green checkmarks appear in the Make Changes column beside all recommendations by default. You can choose which recommendations will be executed by the Assistant by activating or deactivating the checkboxes beside each recommendation.

Browse through each tab in the Dynamics Assistant view to inspect the recommendations.

The Streams tab contains a list of recommendations regarding the setting or removing of pressure-flow specifications in the flowsheet.

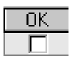
2. Click the **Streams** tab.

Figure 1.145



If some of the columns or rows on the pages are not visible, use the scroll bars beside or under the information area to bring the columns or rows into view.

An active recommendation will be implemented by the Dynamics Assistant.



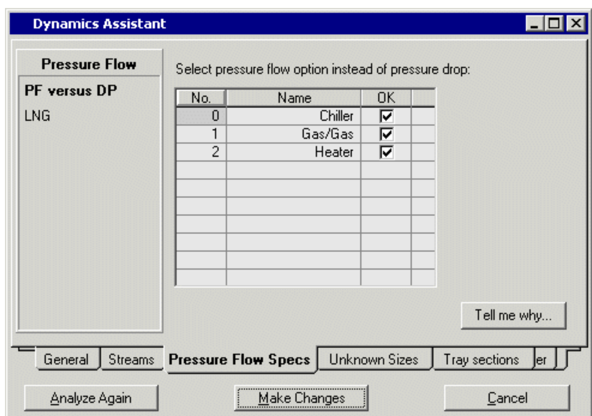
An inactive recommendation will be ignored by the Dynamics Assistant.

3. For each page in the **Streams** tab, set the following recommendations as active or inactive according to the table shown below:

Tab [Page]	Recommendation	Stream	OK Checkbox
Streams [Pressure Specs]	**Remove Pressure Specifications**	Feed 1	Active
	Set Pressure Specifications	LiquidProd	Active
		SalesGas	Active
Streams [Flow Specs]	**Remove Flow Specifications**	Feed 1	Inactive
		Feed 2	Inactive
Streams [Insert Valves]	**Insert Valves**	Feed 1	Inactive
		Feed 2	Inactive
		Ovhd	Inactive
Streams [Int. Flow Spec]	**Set Internal Flow Specification**	Reflux	Active

4. Click the **Pressure Flow Specs** tab.

Figure 1.146



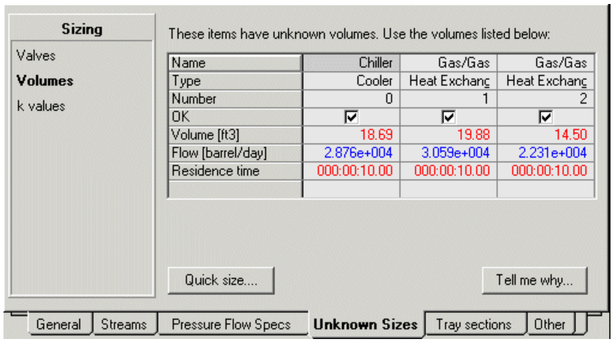
This tab contains a list of unit operations which can use a Pressure Flow or Pressure Drop (DeltaP) specification. Typically, all unit operations in Dynamic mode should use the Pressure Flow specification.

5. Ensure that all the recommendations in this page are active:

Tab [Page]	Recommendation	Unit Operation	OK Checkbox
PressureFlowSpecs [PF versus DP]	**Pressure Flow Spec instead of Delta P**	Chiller	Active
		Gas/Gas	Active
		Heater	Active

6. Click the **Unknown Sizes** tab and select the **Volumes** page.

Figure 1.147



The Unknown Sizes tab contains a list of the unit operations in the flowsheet that require sizing.

- The Valve operations are sized based on the current flow rate and pressure drop across the valve. The valves are sized with a 50% valve opening.
- The Vessel operation volumes are determined based on the liquid exit volumetric flow rate and a 10-second residence time.
- The Heat Exchanger operations are sized based on the current flow rate and pressure drop across the equipment.

You can modify any of the default sizing parameters in the Unknown Sizes tab. Once you modify a sizing parameter, the piece of equipment is automatically sized and the volume, Cv, or k-value displayed.

7. For each page in the **Unknown Sizes** tab, ensure that all the recommendations are active:

Tab [Page]	Recommendation	Unit Operation	OK Checkbox
Unknown Sizes [Volumes]	**Vessel Sizing**	Chiller	Active
		Gas/Gas (Tube) 1	Active
		Gas/Gas (Shell) 2	Active
Unknown Sizes [k values]	**Heat Exchanger Sizing**	Chiller	Active
		Gas/Gas (Tube)	Active
		Gas/Gas (Shell)	Active

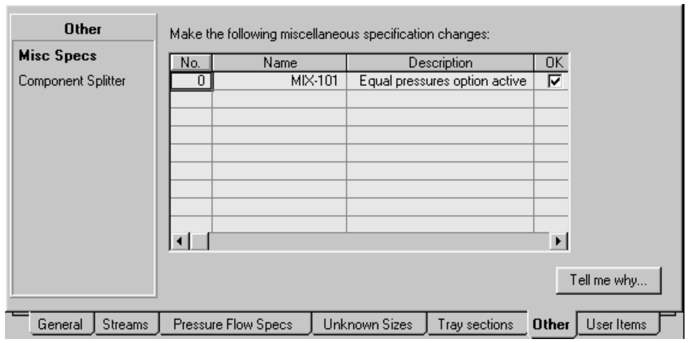
8. Click the **Tray sections** tab.

The Tray sections tab identifies tray sections and streams whose total steady state pressure drops are inconsistent with the total pressure drop calculated according to the dynamics rating model.

For the purpose of this tutorial, recommendations on this tab will be ignored.

9. Click the **Other** tab.

Figure 1.148



The Other tab contains a list of miscellaneous changes that should to be made in order for the Dynamic simulation case to run effectively.

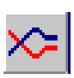
10. Activate the following recommendations:

Tab [Page]	Recommendation	Unit Operation	OK Checkbox
Other [Misc Specs]	**Set Equalize Option Mixers**	Mixer-101	Active

11. Click the **Make Changes** button **once**.

    All the active suggestions in the Dynamics Assistant are implemented.

12. Close the Dynamics Assistant view.



Dynamic Mode icon

13. Switch to Dynamic mode by clicking the **Dynamic mode** icon. When asked “Are you sure you want to switch to dynamics?”, click the **Yes** button.

    Since you deactivated the suggestion to insert a valve on the Ovhd stream, you must set a pressure-flow specification on this stream.

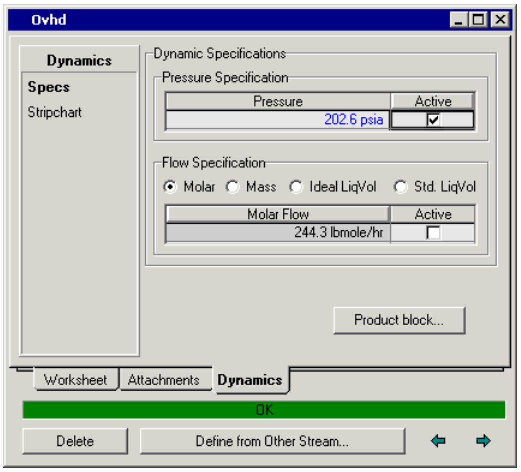
You can enter the Ovhd stream pressure specification in either the Main Flowsheet environment or the Column Sub-Flowsheet.

14. In the PFD, double-click the **Ovhd** stream icon to open stream property view.
15. Click the **Dynamics** tab, then select the **Specs** page.
16. Activate the **Pressure specification** by selecting the appropriate checkbox.

    The Pressure specification should be the only specification active.

Ensure that the Ovhd Molar Flow specification is inactive.

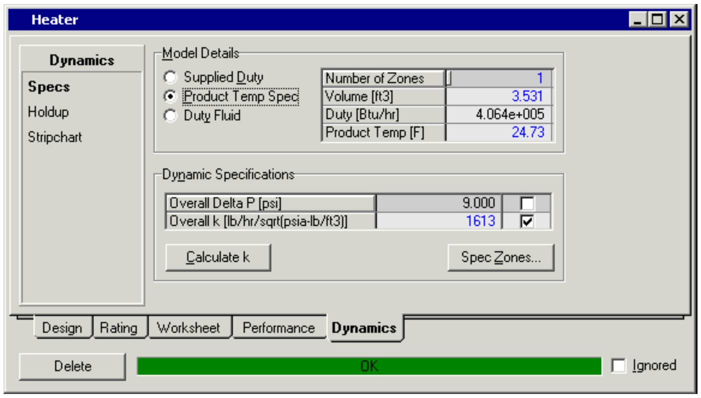
Figure 1.149



17. Close the Ovhd property view.
18. In the PFD, double-click the **Heater** icon to access the property view.
19. Click the **Dynamics** tab, then select the **Specs** page.
20. In the Model Details group, select the **Product Temp Spec** radio button.

You can specify the exit temperature of the Heater operation in Dynamic mode. The duty of the heater is back-calculated to make the temperature specification.

Figure 1.150



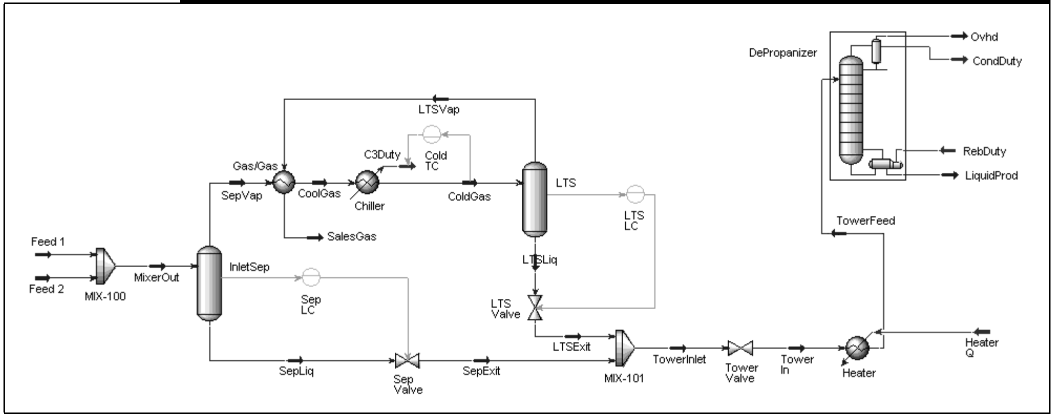
21. Close the view.
22. Save the case as **DynTUT1-3.usc**.

1.3.4 Adding Controller Operations

In this section you will identify and implement key control loops using PID Controller logical operations. Although these controllers are not required to run in Dynamic mode, they will increase the realism of the model and provide more stability.

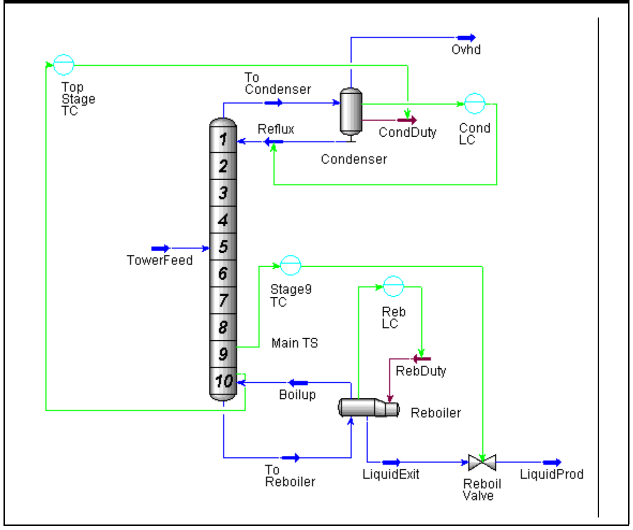
PFD of the main flowsheet environment after all controllers are added:

Figure 1.151



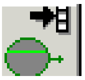
PFD of the Column sub-flowsheet after controllers are added:

Figure 1.152

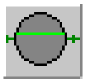


Level Control

In this section you will add level controllers to both the Main flowsheet and Column sub-flowsheet to control the liquid levels of each vessel operation.



Control Ops icon



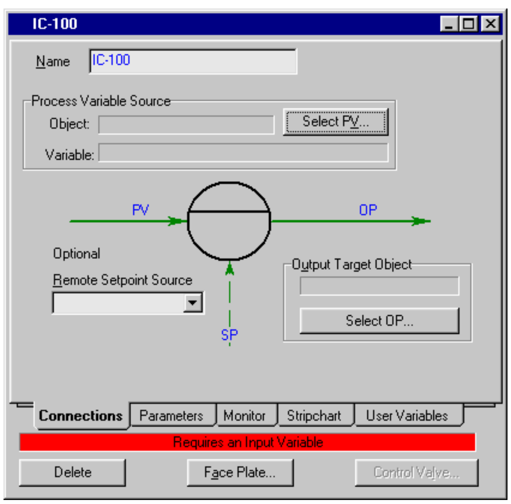
PID Controller icon

1. In the Main flowsheet, access the Object Palette by pressing **F4**.
2. In the Object Palette, click the **Control Ops** icon.

   A sub-palette appears.
3. In the sub-palette, right-click and drag the **PID Controller** icon to the PFD between InletSep and Sep Valve.

   The controller icon **IC-100** appears in the PFD.
4. Double-click the controller icon to open its property view.

Figure 1.153

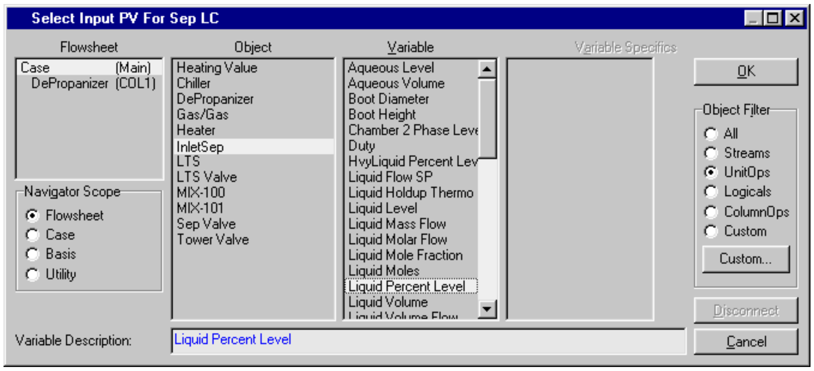


5. Click the **Connections** tab. In the **Name** field, change the name of the PID Controller operation to **Sep LC**.
6. In the Process Variable Source group, click the **Select PV** button.

   The Select Input PV view appears.

7. In the Flowsheet list, select **Case (Main)**. In the Object list, select **InletSep**. In the Variable list, select **Liquid Percent Level**. Click the **OK** button.

Figure 1.154

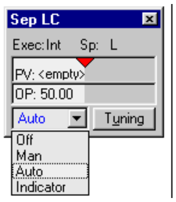


8. In the Output Target Object group, click the **Select OP** button. The Select OP Object view appears.

   The Select OP Object view is exactly the same as the Select Input PV view.

9. In the Flowsheet list, select **Case (Main)**. In the Object list, select **Sep Valve**. In Variable list, select **Actuator Desired position** . Click the **OK** button.
10. Click the **Parameters** tab, then select the **Configuration** page.
11. Enter the information specified in the following table:

In this cell...	Enter...
Action	Select the **Direct** radio button
Kc	2
PV Minimum	0%
PV Maximum	100%



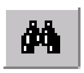
12. Click the **Face Plate** button at the bottom of the property view.
13. Change the controller mode to Auto on the face plate by opening the drop-down list and selecting **Auto**. Close the face plate view when you are finished.

14. Using the same procedures, add another PID Controller operation that will serve as the LTS level controller. Specify the following details:

Tab [Page]	In this cell...	Enter...
Connections	Name	LTS LC
	Process Variable Source	LTS object, Liquid Percent Level variable
	Output Target Object	LTS Valve, Actuator Desired Position
Parameters [Configuration]	Action	Direct
	Kc	2
	PV Minimum	0%
	PV Maximum	100%

15. Click the **Face Plate** button. Change the controller mode to **Auto** on the face plate view.

    Next you will enter the Column sub-flowsheet environment.



Object Navigator icon

16. Instead of entering through the Column property view, click the **Object Navigator** icon in the toolbar.
17. Double-click on DePropanizer in the Flowsheets group to enter the Column sub-flowsheet environment.
18. Ensure the PFD for the column is visible.

The Column sub-flowsheet uses a simplified Object Palette.

To add a PID Controller operation in the sub-flowsheet, right-click the PID Controller icon in the Object Palette and drag the cursor to the PFD.

19. In the Column sub-flowsheet, add a PID Controller operation that will serve as the Condenser level controller. Specify the following details:

Tab [Page]	In this cell...	Enter...
Connections	Name	Cond LC
	Process Variable Source	Condenser, Liquid Percent Level
	Output Target Object	Reflux, Control Valve
Parameters [Configuration]	Action	Direct
	Kc	1
	Ti	5 minutes
	PV Minimum	0%
	PV Maximum	100%

20. Click the **Control Valve** button.

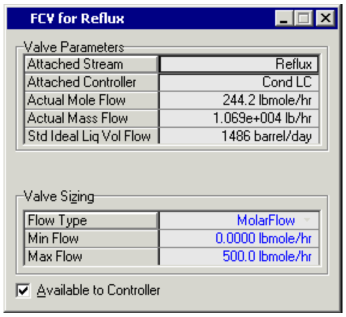
    The FCV for Reflux view appears.

The Flow values shown here do not use the default units. Enter the values, then select the correct units from the drop-down list. UniSim Design automatically converts the values to the default units.

21. Enter the following details in the Valve Sizing group:

In this cell...	Enter...
Flow Type	Molar Flow
Minimum Flow	0 lbmole/h
Maximum Flow	500 lbmole/h

Figure 1.155



22. Close the FCV for Reflux view.
23. Click the **Face Plate** button. Change the controller mode to **Auto** on the face plate view, then close the view.
24. Close the Cond LC controller view.
25. Add another PID Controller operation that will serve as the Reboiler level controller. Specify the following details:

Tab [Page]	In this cell...	Enter...
Connections	Name	Reb LC
	Process Variable Source	Reboiler, Vessel, Liq Percent Level
	Output Target Object	RebDuty, Control Valve
Parameters [Configuration]	Action	Direct
	Kc	0.1
	Ti	3 minutes
	PV Minimum	0%
	PV Maximum	100%

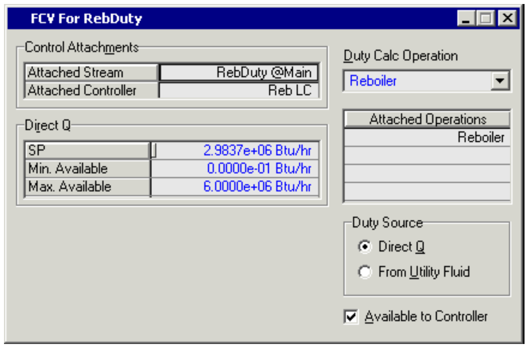
26. Click the **Control Valve** button.

    The FVC for RebDuty view appears.
27. In the Duty Source group, select the **Direct Q** radio button if it is not already selected.
28. In the Direct Q group, enter the following values:

The values shown here do not use the default units. Enter the values, then select the correct units from the drop-down list. UniSim Design automatically converts the values to the default units.

In this cell...	Enter...
Min Available	0 Btu/h
Max Available	6e6 Btu/h

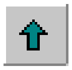
Figure 1.156



29. Close the FCV for RebDuty view.
30. Click the **Face Plate** button. Change the controller mode to **Auto** on the face plate. Close the face plate view.
31. Close the Reb LC property view.

Temperature Control

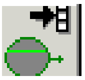
Temperature control is important in this dynamic simulation case. A temperature controller will be placed on the ColdGas stream to ensure that the SalesGas stream makes the **10°F** dewpoint specification. Temperature control will be placed on the top and bottom stages of the depropanizer to ensure product quality and stable column operation.



Enter Parent Simulation Environment icon

1. Enter the Main Flowsheet environment by clicking the **Enter Parent Simulation Environment** button.

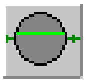
   Next you will add a PID Controller operation that will serve as the ColdGas temperature controller.



Control Ops icon

2. On the Object Palette, click the **Control Ops** icon.

   A sub-palette appears.



PID Controller icon

3. Right-click the **PID Controller** icon, and drag the cursor to the PFD.
4. Double-click the controller icon to open its property view. Specify the following details:

Tab [Page]	In this cell...	Enter...
Connections	Name	Cold TC
	Process Variable Source	ColdGas, Temperature
	Output Target Object	C3Duty, Control Valve

Tab [Page]	In this cell...	Enter...
Parameters [Configuration]	Action	Direct
	Kc	1
	Ti	10 minutes
	PV Minimum	-20 ^{o}F
	PV Maximum	20 ^{o}F

The temperature values shown here do not use the default units. Enter the values, then select the correct units from the drop-down list. UniSim Design automatically converts the values to the default units.

5. Click the **Control Valve** button.

   The FCV for C3Duty appears.
6. In the Duty Source group, select the **Direct Q** radio button.
7. In the Direct Q group, enter the following details:

In this cell...	Enter...
Min Available	0 Btu/h
Max Available	2e6 Btu/h

The values shown here do not use the default units. Enter the values, then select the correct units from the drop-down list. UniSim Design automatically converts the values to the default units.

8. Close the FCV for C3Duty view.
9. Click the **Face Plate** button. Change the controller mode to **Auto** on the face plate view, then close the view.
10. Enter the Depropanizer Column sub-flowsheet environment.
11. Add a PID Controller operation that will serve as the Depropanizer Top Stage temperature controller.
12. In the controller property view, specify the following details:

Tab [Page]	In this cell...	Enter...
Connections	Name	Top Stage TC
	Process Variable Source	Main TS, Top Stage Temperature
	Output Target Object	CondDuty, Control Valve
Parameters [Configuration]	Action	Direct
	Kc	1
	Ti	5 minutes
	PV Minimum	50^{o}F
	PV Maximum	130^{o}F

Ensure that you select the correct temperature units from the units drop-down list.

13. Click the **Control Valve** button.

    The FCV for CondDuty view appears.
14. In the Duty Source group, select the **Direct Q** radio button.
15. in the Direct Q group, enter the following details:

In this cell...	Enter...
Min Available	0 Btu/h
Max Available	3e6 Btu/hr

Ensure that you select the correct units from the units drop-down list.

16. Close the FCV for CondDuty view.
17. Click the **Face Plate** button.

    The Top Stage TC face plate view appears.
18. Change the controller mode to **Auto**. In the **PV** field, enter a set point of **86°F**.
19. Close the Top Stage TC face plate view.
20. Close the Top Stage TC property view.
21. Add another PID Controller operation that will serve as the Depropanizer 9th stage temperature controller.
22. In the controller property view, specify the following details:

Tab [Page]	In this cell...	Enter...
Connections	Name	Stage9 TC
	Process Variable Source	Main TS, Stage Temperature, 9_Main TS
	Output Target Object	Reboil Valve, Actuator Desired position
Parameters [Configuration]	Action	Direct
	Kc	2
	Ti	5 minutes
	PV Minimum	110°F
	PV Maximum	260°F

23. Click the **Face Plate** button.

    The Stage 9 TC face plate view appears.

Ensure that you select the correct temperature units from the units drop-down list.

24. Change the controller mode to **Auto**. In the **PV** field, input a set point of **184°F**.

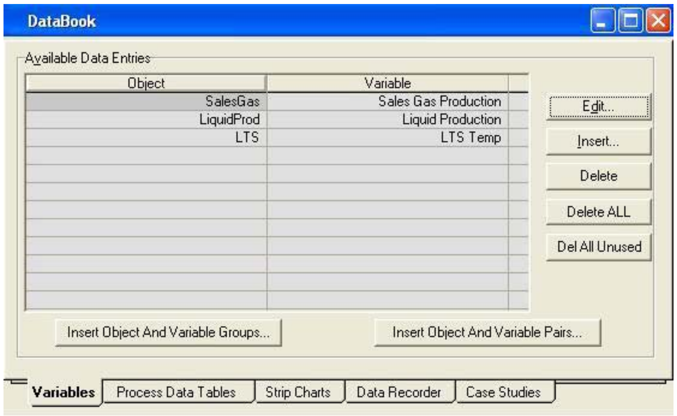
    You should be able to run the integrator at this point without any problems, however, you will probably want to monitor important variables in the dynamic simulation using strip charts.
25. Return to the Parent Environment.
26. Save the case as **DynTUT1-4.usc**.

Monitoring in Dynamics

Now that the model is ready to run in Dynamic mode, you will create a strip chart to monitor the general trends of key variables. The following is a general procedure for installing strip charts in UniSim Design.

1. Open the Databook by using the hot key combination **CTRL D**.

Figure 1.157



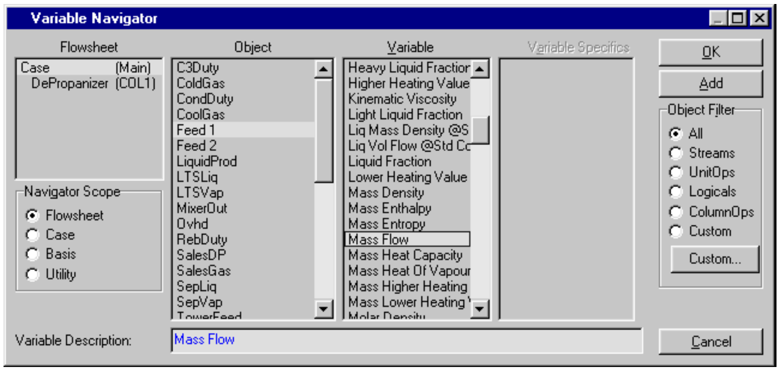
For more information, refer to **Using the Databook** on page 70.

In the next set of steps, you will add all of the variables that you would like to manipulate or model.

- Include feed and energy streams that you want to modify in the dynamic simulation.
- Include unit operation temperature, levels, and pressures that you want to monitor and record.

2. On the **Variables** tab, click the **Insert** button. The Variable Navigator appears.

Figure 1.158



Select Case (Main) in the Flowsheet group to ensure you can find all streams and operations.

3. Select the Object and Variable groups for any of the following suggested variables.

Object	Variable
Tower Feed	Molar Flow
Heater Q	Utility outlet Temp
Feed 1	Molar Flow
Feed 2	Molar Flow

Object	Variable
Ovhd	Molar Flow
LiquidProd	Molar Flow
InletSep	Liquid Percent Level
LTS	Liquid Percent Level

4. Click the **Add** button to add the selected variable to the **Variables** page.

The purpose of selecting manipulated and monitored objects is to see how the monitored objects will respond to the changes you make to the manipulated variable.

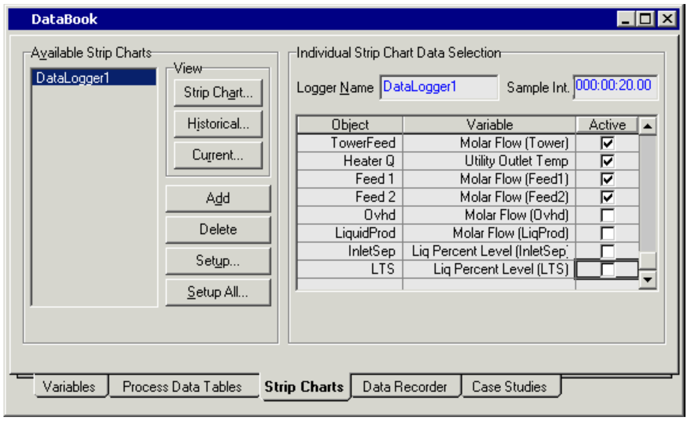
5. Repeat steps #3 and #4 to add any remaining variables to the Databook.
6. Click the **Strip Charts** tab.
7. In the Available Strip Charts group, click the **Add** button.

   UniSim Design will create a new strip chart with the default name DataLogger1. You may change the default name by editing the Logger Name cell.

To make the strip chart easier to read, do not activate more than six variables per strip chart.

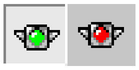
8. In the table, check the **Active** checkbox for each of the variables that you would like to monitor on this particular strip chart.

Figure 1.159



To change the configuration of each strip chart, click the **Setup** button.

9. If required, add more strip charts by repeating steps #7 and #8.
10. To access a strip chart view, select the strip chart name, then click the **Strip Chart** button.
11. Minimize the Databook view.
12. Before starting the integrator, open the property view for the **Ovhd** stream.
13. Click the **Dynamics** tab, then select the **Specs** page.
14. In the Dynamic Specifications group, ensure that the Pressure specification checkbox is **Active** and the Molar Flow specification checkbox is **Inactive**.
15. Close the Ovhd stream view.



Start Integrator icon (green)

16. Arrange both strip chart views so you can see them.
17. Start the Integrator by clicking the **Start Integrator** icon in the tool bar and observe as the variables line out on the strip charts.
18. Click the **Stop Integrator** icon to stop the process.

    To use the Databook feature for analysis, manipulate the stream and operation variables via their property views, click the **Start Integrator** icon again, and view the results in the monitored variables in the strip charts.

2 Refining Tutorial

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2.1 Introduction

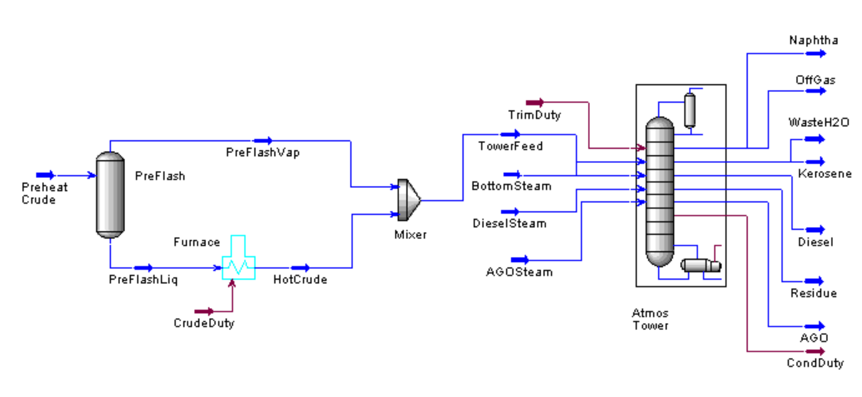
You will build the Refining simulation using the following basic steps:

1. Create a unit set.
2. Choose a property package.
3. Select the non-oil components.
4. Characterize the Oil.
5. Create and specify the preheated crude and utility steam streams.
6. Install and define the unit operations in the pre-fractionation train.
7. Install and define the crude fractionation column.

This complete case has also been pre-built and is located in the file **TUTOR2.usc** in your UniSim Design\Samples directory.

In this tutorial, crude oil is processed in a fractionation facility to produce naphtha, kerosene, diesel, atmospheric gas oil, and atmospheric residue products. Preheated crude (from an upstream preheat train) is fed to a pre-flash drum where vapours are separated from the liquids, which are heated in a furnace. The pre-flash vapours bypass the furnace and are recombined with the hot crude from the furnace. The combined stream is then fed to the atmospheric crude column for fractionation. The main flowsheet for this process appears below.

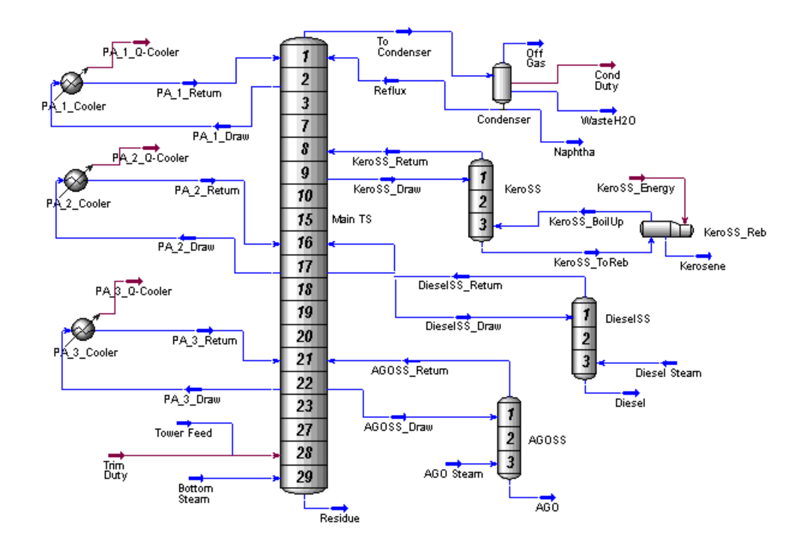
Figure 2.1



The crude column consists of a refluxed absorber with three side strippers and three cooled pump around circuits. The column sub-

flowsheet appears below.

Figure 2.2



The following pages guide you through building a UniSim Design case for modeling this process. This tutorial illustrates the complete construction of the simulation, from selecting a property package and components, characterizing the crude oil, to installing streams and unit operations, through to examining the final results. The tools available in UniSim Design are utilized to illustrate the flexibility available to you.

Before proceeding, you should have read Chapter A - UniSim Design Tutorials which precedes the Tutorials in this guide.

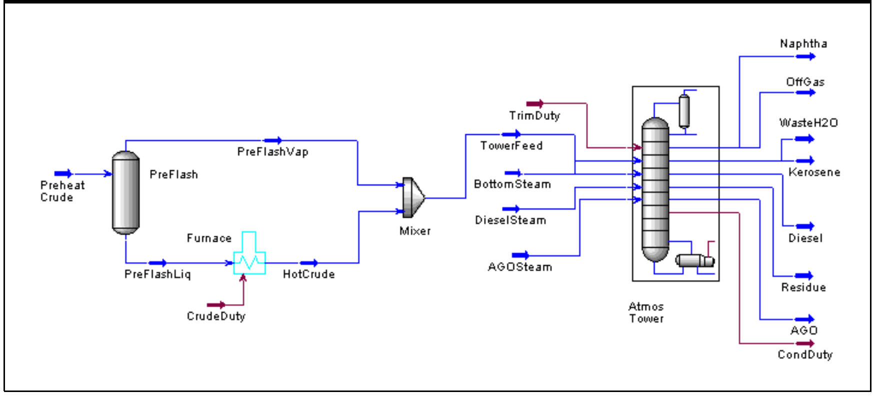
2.2 Steady State Simulation

2.2.1 Process Description

This example models a crude oil processing facility consisting of a pre-fractionation train used to heat the crude liquids, and an atmospheric crude column to fractionate the crude into its straight run products. The

Main Flowsheet for this process appears in the following figure.

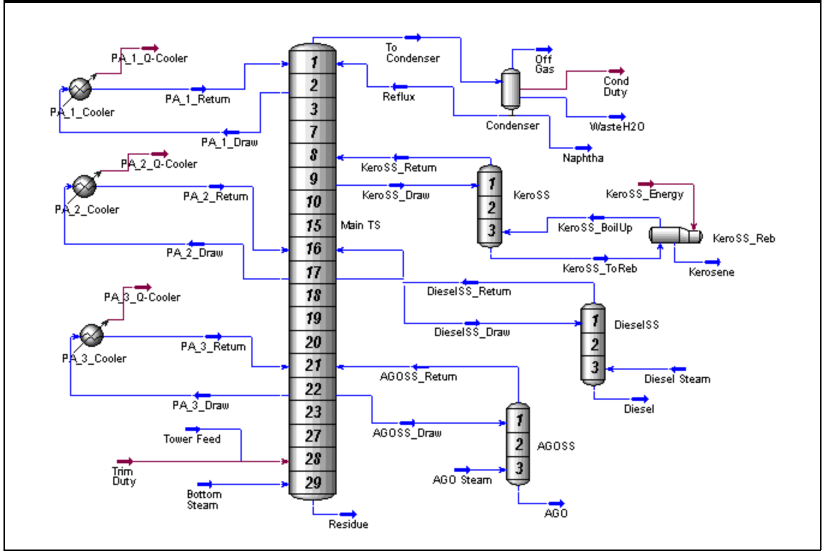
Figure 2.3



Preheated crude (from a preheat train) is fed to the pre-flash drum, modeled as a Separator, where vapours are separated from the crude liquids. The liquids are then heated to 650°F in the crude furnace, modeled as a Heater. The pre-flash vapours bypass the furnace and are re-combined, using a Mixer, with the hot crude stream. The combined stream is then fed to the atmospheric crude column for separation.

The crude column is modeled as a Refluxed Absorber, equipped with three pump-around and three side stripper operations. The Column sub-flowsheet appears in the figure below.

Figure 2.4



The main column consists of 29 trays plus a partial condenser. The TowerFeed enters on stage 28, while superheated steam is fed to the bottom stage. In addition, the trim duty is represented by an energy

stream feeding onto stage 28. The Naphtha product, as well as the water stream WasteH2O, are produced from the three-phase condenser. Crude atmospheric Residue is yielded from the bottom of the tower.

Each of the three-stage side strippers yields a straight run product. Kerosene is produced from the reboiled KeroSS side stripper, while Diesel and AGO (atmospheric gas oil) are produced from the steam-stripped DieselSS and AGOSS side strippers, respectively.

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.

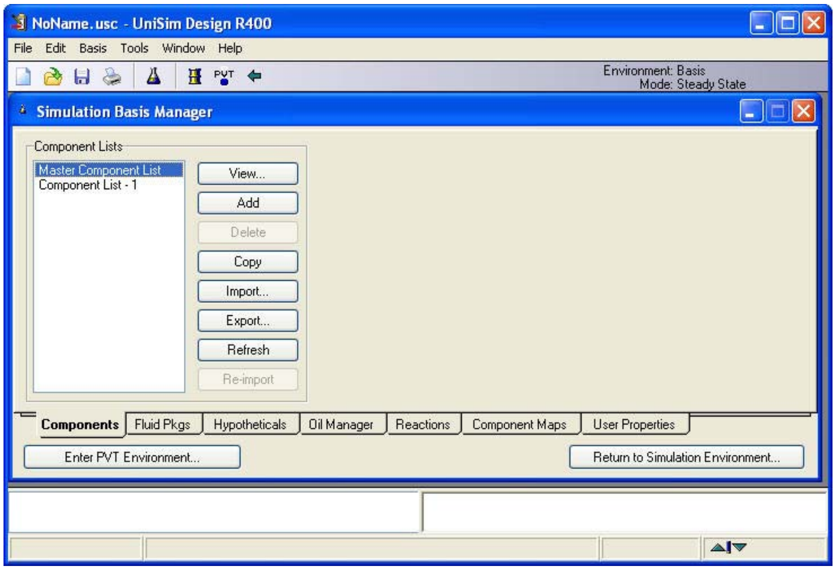
The Workbook is used to build the first part of the flowsheet, from specifying the feed conditions through to installing the pre-flash separator. The PFD is then used to install the remaining operations, from the crude furnace through to the column.

2.2.2 Setting Your Session Preferences

1. Start UniSim Design and create a new case. The Simulation Basis

Manager view appears.

Figure 2.5



The default Preference file is named **UniSim Design R*.prf**. When you modify any of the preferences, you can save the changes in the default file by clicking Save Preferences, or in a new preference file by clicking the **Save Preference As...** . UniSim Design prompts you to provide a name for the new Preference file, which you can later use in any simulation case by clicking the **Load Preferences** button.

Your first task is to set your Session Preferences.

2. From the **Tools** menu, select **Preferences**.

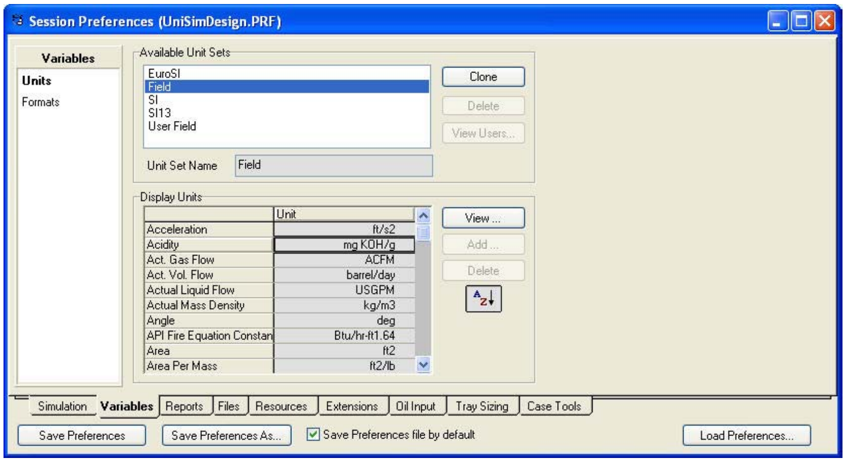
   The Session Preferences view appears.

   The most important preference you will set is the unit set. UniSim Design does not allow you to change any of the default unit sets listed, however, you can create a new unit set by cloning an existing one. In this tutorial you will create a new unit set based on the UniSim Design Field set and customize it.

3. Click the **Variables** tab, then select the **Units** page.

4. In the Available Unit Sets group, select **Field**.

Figure 2.6



5. Click the **Clone** button.

   A new unit set named NewUser appears and is automatically selected as the current unit set.

6. In the **Unit Set Name** field, rename the new unit set to **Field-density**.

   You can now change the units for any variable associated with this new unit set.

7. In the Display Units group, use the vertical scroll bar to find the **Standard Density** cell.

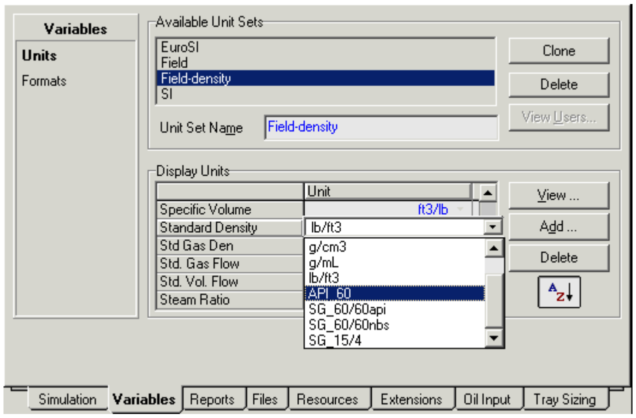
   The current default unit for **Standard Density** is lb/ft3. A more appropriate unit for this example is API_60.

8. Click in the **Standard Density** cell on lb/ft3.

9. Press the **SPACEBAR** or the **DOWN** arrow to open the drop-down list of available units.

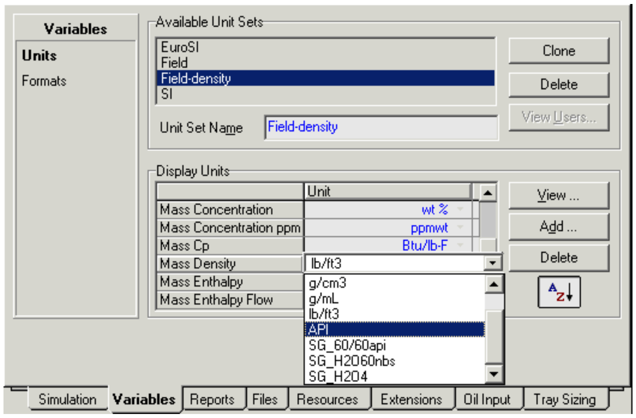
10. In the unit list, select **API_60**.

Figure 2.7



11. Repeat steps #8-#10 to change the **Mass Density** units to **API**.

Figure 2.8



All commands accessed via the toolbar are also available as Menu items.

12. Your new unit set is now defined. Close the Session Preference view to return to the Simulation Basis Manager view.

2.2.3 Building the Simulation

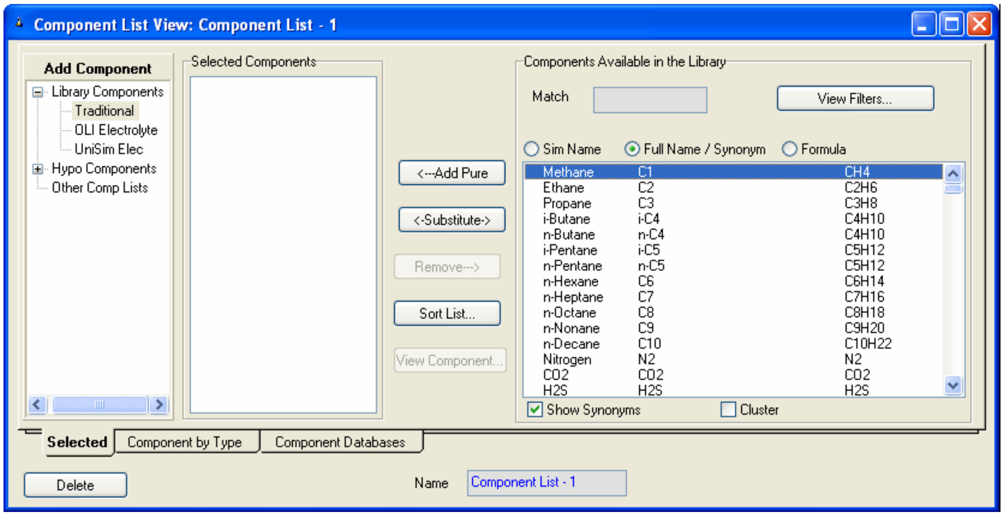
Selecting Components

Before defining a fluid package in UniSim Design, you will create a component list for the fluid package. In this example, the component list contains non-oil components, Light Ends, and hypocomponents. You must first add the non-oil components and Light Ends from UniSim

Design pure component library into the component list.

1. Click the **Components** tab, then click the **Add** button. The Component List View view appears.

Figure 2.9



There are a number of ways to select components for your simulation. One method is to use the matching feature.

Notice that each component is listed in three ways on the Selected tab:

Matching Method	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.

The Component List View view contains two tabs. In this example, the Selected tab is the only tab used, because it contains all the functions you need to add components to the list.

At the top of each of these three columns is a corresponding radio button. Based on the selected radio button, UniSim Design will locate the component(s) that best matches the input you type in the **Match** cell.

2. Optional: To rename the component list, click in the **Name** field at the bottom of the view and type a new name.

   For this tutorial example, you will add the following non-oil components: H2O, C3, i-C4, n-C4, i-C5 and n-C5.

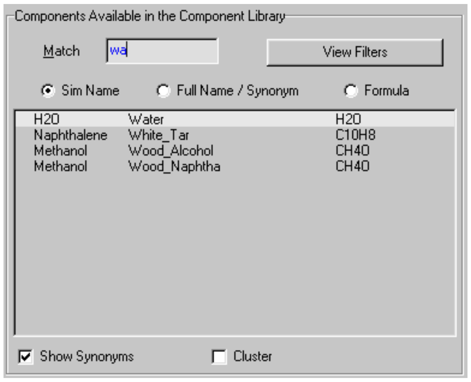
   First, you will add **H2O** using the match feature.

3. Ensure the **Sim Name** radio button is selected, and the **Show Synonyms** checkbox is checked.

You can also move to the Match field by pressing **ALT M**.

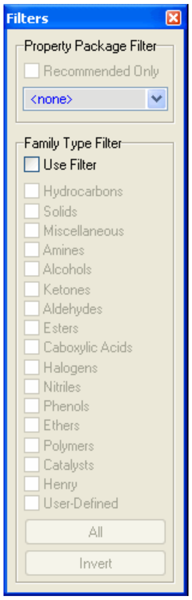
4. Click in the **Match** field.
5. Begin typing 'water'. UniSim Design filters through its library as you type, displaying only those components that match your input.

Figure 2.10



6. With Water selected, add it to the Current Component List by doing **one** of the following:
   - Press the **ENTER** key.
   - Click the **Add Pure** button.
   - Double-click on Water.

   You can also use the Family Filter to display only those components belonging to certain families. Next, you will add Propane to the component list using a Family Filter:



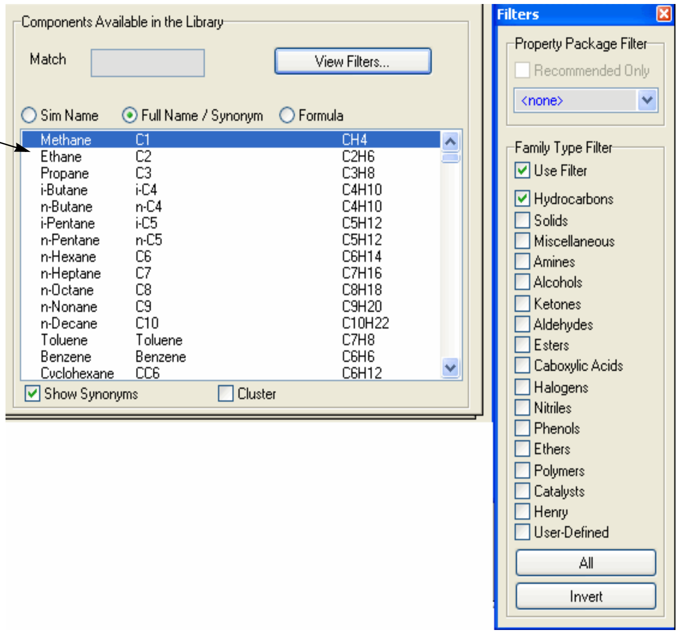
Filters view

7. Ensure the **Match** field is empty, and click the **View Filter** button. The Filters view appears as shown on the left.
8. On the Filters view, check the **Use Filter** checkbox to activate the Family Filter.

9. Check the **Hydrocarbons** checkbox. The remaining components are known to be hydrocarbons.

Figure 2.11

On the Component View view, Propane appears near the top of the filtered list.



The Match feature remains active when you are using a family filter, so you could have also typed **C3** in the Match field and then added it to the component list.

10. Double-click Propane to add it to the component list.

    Next you will add the remaining Light Ends components i-C4 through n-C5. The following procedure shows you quick way to add components that appear consecutively in the library list.

11. Click on the first component to be added (in this case, i-C4).

12. Do **one** of the following:

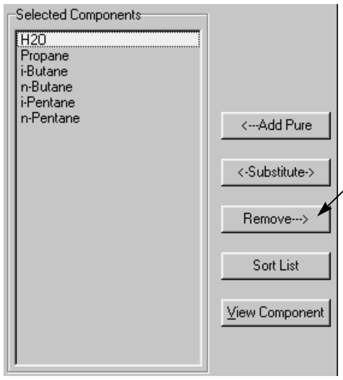
To select consecutive components, use the **SHIFT** key.

To select non-consecutive components, use the **CTRL** key.

- Hold down the **SHIFT** key and click on the last component, in this case n-C5. All components i-C4 through n-C5 are now selected. Release the **SHIFT** key.
- Click and drag from i-C4 to n-C5. Components i-C4 through to n-C5 are selected.

13. Click the **Add Pure** button. The selected components are transferred to the Selected Component group.

Figure 2.12



To remove a component from the Current Components List, select it and click the Remove button or press the **DELETE** key.

The complete list of non-oil components appears in the figure above.

14. Close the Component List View and Filters views to return to the Simulation Basis Manager view.

On the Components tab, the Component Lists group now contains the name of the new component list that you created.

Defining a Fluid Package

In the Simulation Basis Manager view, your next task is to define a fluid package.

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 require only one fluid package for your entire simulation.

UniSim Design 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 choose the property package and non-oil components.

A fluid package contains the components and property methods that UniSim Design will use in its calculations for a particular flowsheet. Depending on what is required, a fluid package can also contain other information, such as a petroleum fluid characterization.

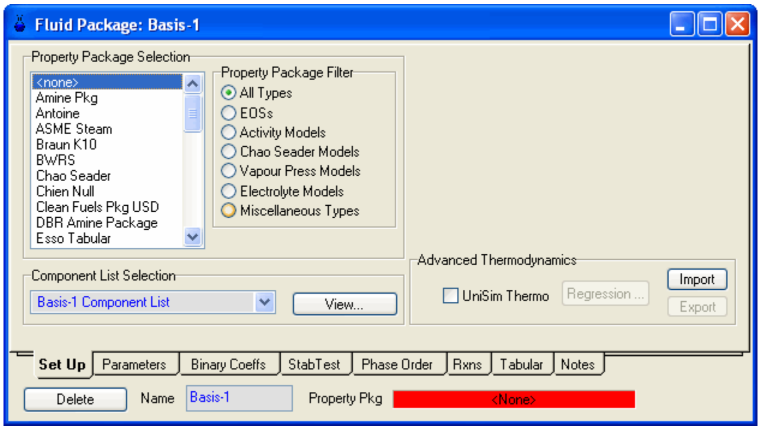
UniSim Design has created a fluid package with the default name Basis-1. You can change the name of this fluid package by typing a new name in the **Name** field at the bottom of the view.

The fluid package for this example will contain the property package (Peng Robinson), the pure components H2O, C3, i-C4, n-C4, i-C5, n-C5, and the hypothetical components which are generated in the Oil characterization.

1. Click the **Fluid Pkgs** tab, then click the **Add** button. The Fluid

Package: Basis-1 view appears.

Figure 2.13



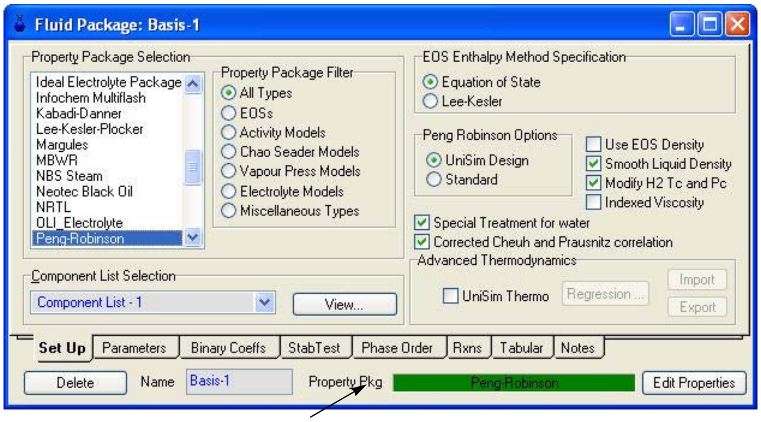
This view is divided into a number of tabs that allow you to supply all the information necessary to completely define the fluid package. For this tutorial, however, only the Set Up tab is used.

On the Set Up tab, the currently selected Property Package is <none>. Before you begin characterizing your petroleum fluid, you must choose a property package that can handle hypothetical components.

2. Select the Peng Robinson property package by doing **one** of the following:
   - Type **Peng Robinson**. UniSim Design finds the match to your input.
   - Use the up and down arrow keys to scroll through the list of available property packages until Peng Robinson is selected.
   - Use the vertical scroll bar to scroll through the list until Peng Robinson becomes visible, then click on it.

The Fluid Package: Basis - 1 view appears as shown below.

Figure 2.14



The Property Pkg indicator now indicates **Peng Robinson** is the current property package for this fluid package.

Alternatively, you could have selected the EOSs radio button in the Property Pkg Filter group. The list would then display only those property packages that are Equations of State. Peng Robinson would appear in this filtered list.

If you have multiple fluid packages and components lists in a case, you can use the drop-down list in the Component List Selection group to attache a component list to a particular property package.

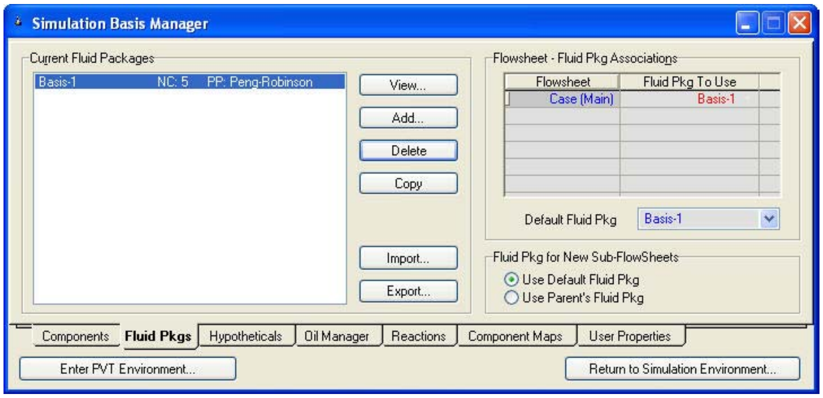
In the Component List Selection group, you could use the drop-down list to find the name of any component lists you had created (currently empty).

The View button opens the Component List View view of the selected component list.

If the selected component list contains components not appropriate for the selected property package, UniSim Design opens the Components Incompatible with Property Package view. On this view, you have the options of UniSim Design removing the incompatible components from the component list or changing to a different property package using the drop-down list or the Cancel button.

3. Close the Fluid Package: Basis - 1 view to return to the Simulation Basis Manager view.

Figure 2.15



The list in the Current Fluid Packages group 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 flowsheet, as shown in the Flowsheet-Fluid Pkg Associations group.

Creating Hypocomponents

Your next task is to create and add the hypocomponents to the component list. In this example, you will characterize the oil (Petroleum Fluid) using the given Assay data to create the hypocomponents.

Characterizing the Oil

In this section, you will use the following laboratory Assay data:

Bulk Crude Properties	
MW	300.00
API Gravity	48.75

Light Ends Liquid Volume Percent	
i-Butane	0.19
n-Butane	0.11
i-Pentane	0.37
n-Pentane	0.46

TBP Distillation Assay		
Liquid Volume Percent Distilled	**Temperature (°F)**	**Molecular Weight**
0.0	80.0	68.0
10.0	255.0	119.0
20.0	349.0	150.0
30.0	430.0	182.0
40.0	527.0	225.0
50.0	635.0	282.0
60.0	751.0	350.0
70.0	915.0	456.0
80.0	1095.0	585.0
90.0	1277.0	713.0
98.0	1410.0	838.0

API Gravity Assay	
Liq Vol% Distilled	**API Gravity**
13.0	63.28
33.0	54.86
57.0	45.91
74.0	38.21
91.0	26.01

Viscosity Assay		
Liquid Volume Percent Distilled	**Viscosity (cP) 100°F**	**Viscosity (cP) 210°F**
10.0	0.20	0.10
30.0	0.75	0.30
50.0	4.20	0.80
70.0	39.00	7.50
90.0	600.00	122.30

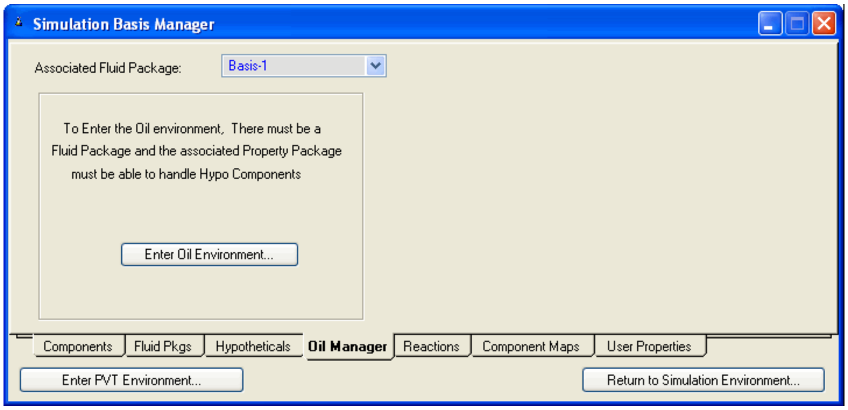
Accessing the Oil Environment

The UniSim Design Oil Characterization procedure is used to convert the laboratory data into petroleum hypocomponents.

The Associated Fluid Package drop-down list indicates which fluid package is used for the oil characterization. Since there is only one fluid package, UniSim Design has made **Basis-1** the Associated Fluid Package.

1. On the Simulation Basis Manager view, click the **Oil Manager** tab.

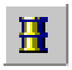
Figure 2.16



The text on the right side of the view indicates that before entering the Oil Environment, two criteria must be met:

- at least one fluid package must be present. In this case, only one fluid package, Basis-1, is selected.
- the property package must be able to handle Hypothetical Components. In our case, the property package is Peng Robinson, which is capable of handling Hypothetical components.

Since both criteria are satisfied, the oil is characterized in the Oil Environment.



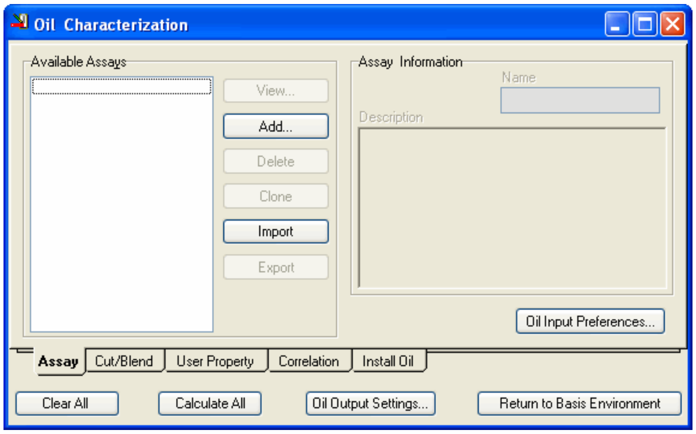
Oil Environment icon

The Oil Characterization view allows you to create, modify, and otherwise manipulate the Assays and Blends in your simulation case. For this example, the oil is characterized using a single Assay.

2. To enter the Oil Characterization environment, do **one** of the following:
   - click the **Enter Oil Environment** button on the Oil Manager tab.
   - click the **Oil Environment** icon on the toolbar.

The Oil Characterization view appears.

Figure 2.17



In general, three steps must be completed when you are characterizing a petroleum fluid:

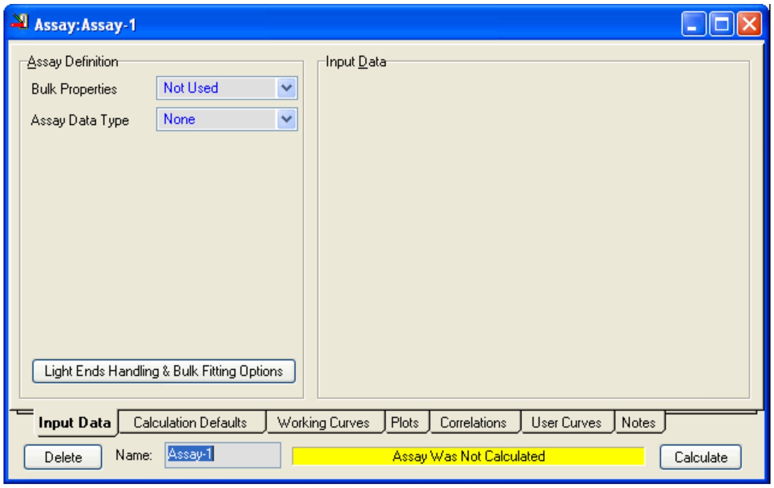
1. Supply data to define the Assay.
2. Cut the Assay into hypothetical components by creating a Blend.
3. Install the hypothetical components into the fluid package.

Defining the Assay

UniSim Design has given the new Assay the default name of Assay-1. You can change this by typing a new name in the **Name** field.

1. On the **Assay** tab, click the **Add** button to create and view a new Assay. The Assay view appears.

Figure 2.18

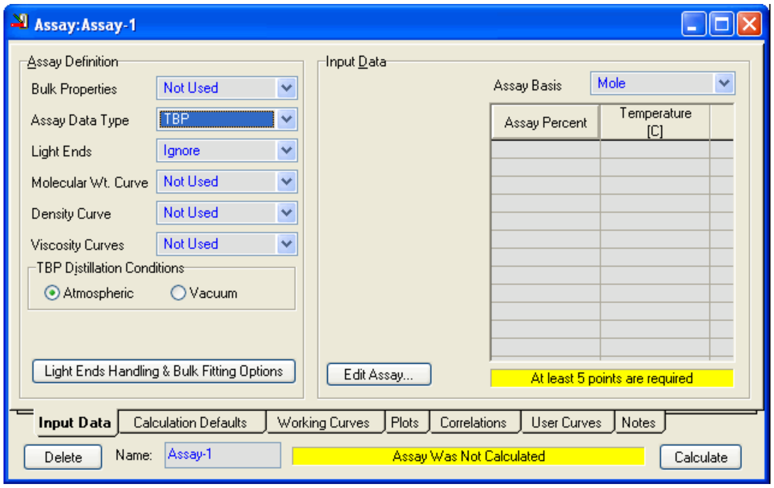


When the property view for a new Assay is opened for the first time,

the view contains minimal information. Depending on the Assay Data Type you choose, the view is modified appropriately. For this example, the Assay is defined based on TBP data.

2. From the Assay Data Type drop-down list, select TBP. The view is customized for TBP data.

Figure 2.19

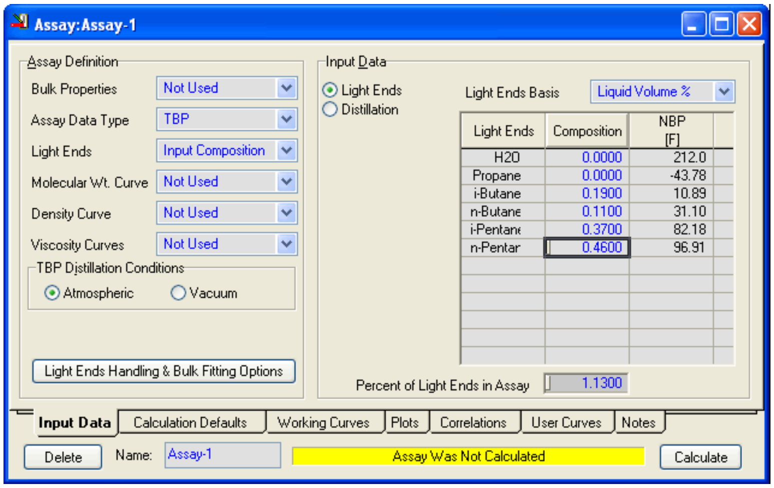


The next task is to enter the composition of the Light Ends in the Assay.

3. From the Light Ends drop-down list, select Input Composition.
4. In the Input Data group, select the **Light Ends** radio button.
5. Ensure that Liquid Volume% is selected in the Light Ends Basis drop-down list.
6. Click in the **Composition** cell for i-Butane.
7. Type 0.19, then press the **ENTER** key. You are automatically advanced down one cell to n-Butane**.**

8. Type the remaining compositions as shown. The total Percent of Light Ends in Assay is calculated and displayed at the bottom of the table.

Figure 2.20



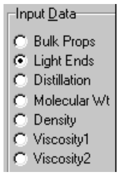
Before entering any of the assay data, you must activate the molecular weight, density, and viscosity curves by choosing appropriate curve types in the Assay Definition group. Currently, these three curves are not used.

9. From the Bulk Properties drop-down list, select Used. A new radio button labeled **Bulk Props** appears in the Input Data group.

10. From Molecular Wt. Curve drop-down list, select Dependent. A new radio button labeled **Molecular Wt** appears in the Input Data group.

11. From the Density Curve and Viscosity Curves drop-down lists, select Independent as the curve type. For Viscosity, two radio buttons appear as UniSim Design allows you to input viscosity assay data at two temperatures.

    Your view now contains a total of seven radio buttons in the Input Data group. The laboratory data are input in the same order as the radio buttons appear.



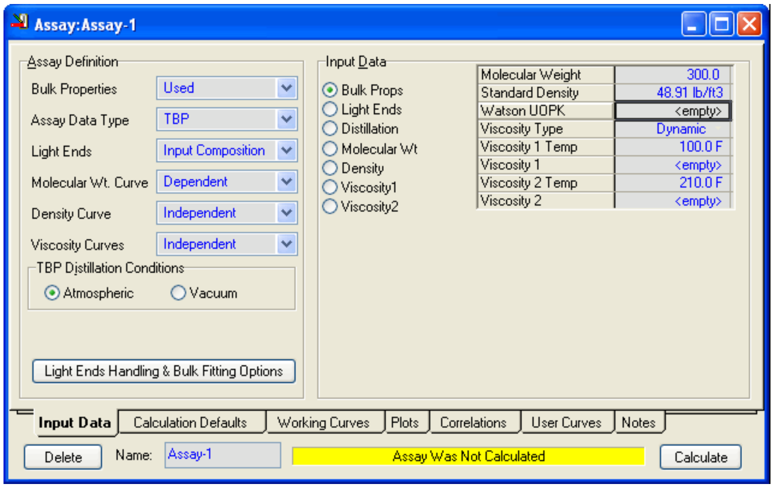
In the next few sections, you will enter the following laboratory assay data:

- bulk molecular weight and density
- TBP Distillation assay data
- dependent molecular weight assay data
- independent density assay data
- independent viscosity assay data (at two temperatures)

Entering Bulk Property Data

1. Select the **Bulk Props** radio button, and the bulk property table appears to the right of the radio buttons.
2. Click in the **Molecular Weight** cell in the table. Type 300 and press **ENTER**. You are automatically advanced down one cell to the **Standard Density** cell.
3. In the **Standard Density** cell, enter 48.75 and press **SPACE BAR**. To the right of the cell, a field containing the current default unit associated with the cell appears. When you defined the new unit set, you specified the default unit for standard density as API_60, which appears in the field.

Figure 2.21



4. Since this is the correct unit, press **ENTER**, and UniSim Design accepts the density value.

   No bulk Watson UOPK or Viscosity data is available for this assay. UniSim Design provides two default temperatures (100°F and 210°F) for entering bulk viscosity, but these temperature values are ignored unless corresponding viscosities are provided. Since the value for bulk viscosity is not supplied, there is no need to delete or change the temperature values.

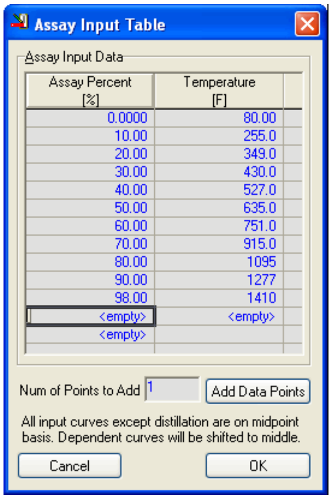
Entering Boiling Temperature (TBP) Data

The next task is to enter the TBP distillation data.

1. Click the **Calculation Defaults** tab.
2. In the Extrapolation Methods group, select Lagrange for each method using the drop-down lists.
3. Return to the **Input Data** tab.

4. Select the **Distillation** radio button. The corresponding TBP data matrix appears. UniSim Design displays a message under the matrix, stating that ‘At least 5 points are required’ before the assay can be calculated.
5. From the Assay Basis drop-down list, select **Liquid Volume**.
6. Click the **Edit Assay** button. The Assay Input Table view appears.
7. Click in the top cell of the Assay Percent column.
8. Type **0** then press **ENTER**. You are automatically advanced to the corresponding empty Temperature cell.
9. Type **80** then press **ENTER**. You are automatically advanced down to the next empty Assay Percent cell.
10. Repeat steps #8 and #9 to enter the remaining Assay Percent and Temperature values as shown.

Figure 2.22



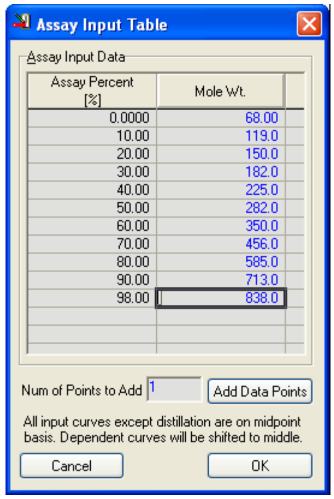
11. Click the **OK** button to return to the Assay property view.

Entering Molecular Weight Data

1. Select the **Molecular Wt** radio button. The corresponding assay matrix appears. Since the Molecular Weight assay is Dependent, the Assay Percent column displays the same values as those you entered for the Boiling Temperature assay. Therefore, you need only enter the Molecular Weight value for each assay percent.
2. Click the **Edit Assay** button and the Assay Input Table view appears.
3. Click on the first empty cell in the Mole Wt column.
4. Type 68, then press the down arrow key.

5. Type the remaining Molecular Weight values as shown.

Figure 2.23

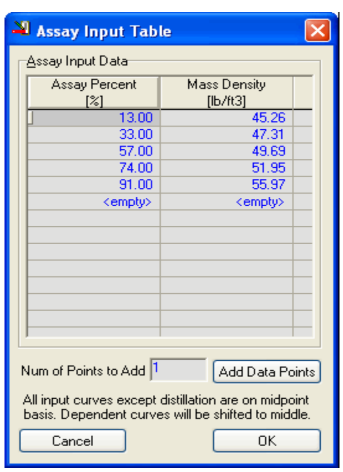


6. Click the **OK** button when you are finished.

Entering Density Data

1. Select the **Density** radio button. The corresponding assay matrix appears. Since the Density assay is Independent, you must input values in both the **Assay Percent** and **Density** cells.
2. Using the same method as for the previous assays, enter the API gravity curve data as shown here.

Figure 2.24

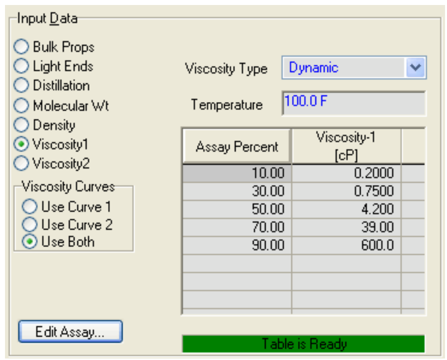


Entering Viscosity Data

1. Select the **Viscosity 1** radio button. The corresponding assay matrix appears.
2. In the Viscosity Type drop-down list above the assay matrix, ensure Dynamic is selected.
3. In the Viscosity Curves group, select the **Use Both** radio button. The Temperature field is for each of the two viscosity curves.
4. Input the Viscosity 1 assay data as shown here. This viscosity curve corresponds to Temperature 1, 100°F.

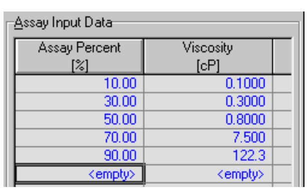
Click the **Edit Assay** button to access the Assay Input Table.

Figure 2.25



5. Select the **Viscosity 2** radio button.
6. Enter the assay data corresponding to Temperature 2, 210°F, as shown.

Figure 2.26

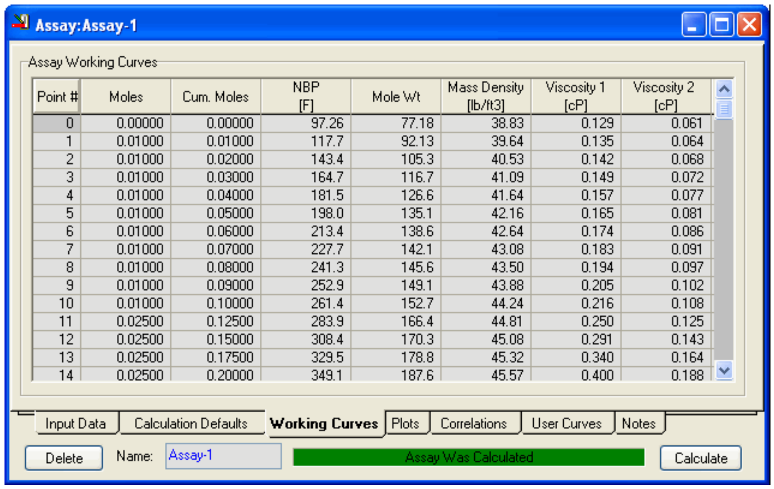


The Assay is now completely defined based on our available data.

7. Click the **Calculate** button at the bottom of the Assay view. UniSim Design calculates the Assay, and the status message at the bottom of the view changes to Assay Was Calculated.

8. Click the **Working Curves** tab of the Assay property view to view the calculated results.

Figure 2.27

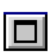


Point #	Moles	Cum. Moles	NBP [F]	Mole Wt	Mass Density [lb/ft3]	Viscosity 1 [cP]	Viscosity 2 [cP]
0	0.00000	0.00000	97.26	77.18	38.83	0.129	0.061
1	0.01000	0.01000	117.7	92.13	39.64	0.135	0.064
2	0.01000	0.02000	143.4	105.3	40.53	0.142	0.068
3	0.01000	0.03000	164.7	116.7	41.09	0.149	0.072
4	0.01000	0.04000	181.5	126.6	41.64	0.157	0.077
5	0.01000	0.05000	198.0	135.1	42.16	0.165	0.081
6	0.01000	0.06000	213.4	138.6	42.64	0.174	0.086
7	0.01000	0.07000	227.7	142.1	43.08	0.183	0.091
8	0.01000	0.08000	241.3	145.6	43.50	0.194	0.097
9	0.01000	0.09000	252.9	149.1	43.88	0.205	0.102
10	0.01000	0.10000	261.4	152.7	44.24	0.216	0.108
11	0.02500	0.12500	283.9	166.4	44.81	0.250	0.125
12	0.02500	0.15000	308.4	170.3	45.08	0.291	0.143
13	0.02500	0.17500	329.5	178.8	45.32	0.340	0.164
14	0.02500	0.20000	349.1	187.6	45.57	0.400	0.188

UniSim Design has calculated 50 points for each of the Assay Working Curves.

The plot view can be re-sized to make the plot more readable. To re-size the view, do **one** of the following:

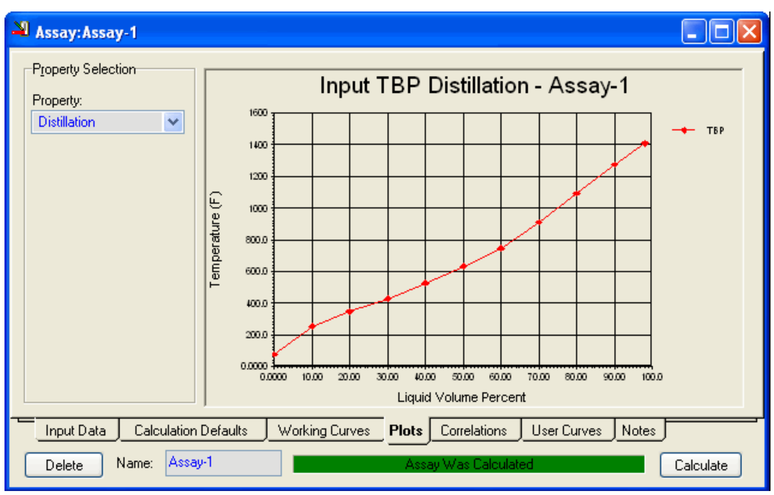
- Click and drag the outside border to the new size.
- Click the **Maximize** icon.



Maximize icon

9. To view the Assay data you input in a graphical format, click the **Plots** tab. The input curve that appears is dependent on the current variable in the Property drop-down list. By default, UniSim Design plots the Distillation (TBP) data. This plot appears below.

Figure 2.28



The independent (x-axis) variable is the Assay percent, while the dependent variable is the TBP in °F. You can view any of the other input curves by selecting the appropriate variable in the Property drop-down list.

The remaining tabs in the Assay property view provide access to information which is not required for this tutorial.

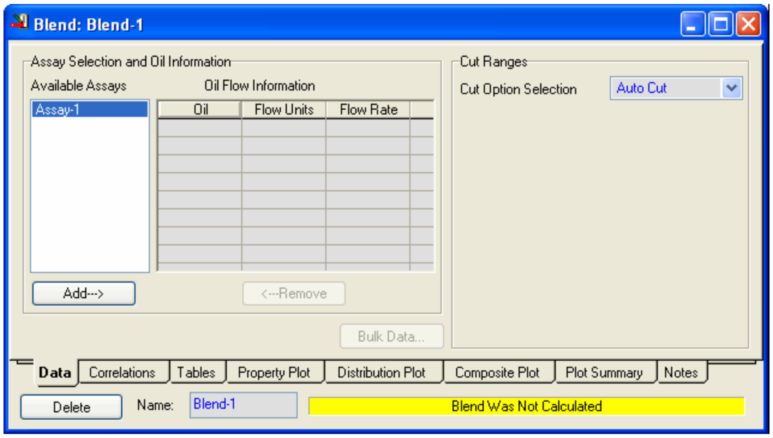
10. Close the Assay view to return to the Oil Characterization view.

Cutting the Assay (Creating the Blend)

Now that the assay has been calculated, the next task is to cut the assay into individual petroleum hypocomponents.

1. Click the **Cut/Blend** tab of the Oil Characterization view.
2. Click the **Add** button. UniSim Design creates a new Blend and displays its property view.

Figure 2.29



3. In the list of Available Assays, select Assay-1.
4. Click the **Add** button. There are two results:
   - The Assay is transferred to the Oil Flow Information table. (When you have only one Assay, there is no need to enter a Flow Rate in this table.)
   - A Blend (Cut) is automatically calculated based on the current Cut Option.

   In this case, the Blend was calculated based on **Auto Cut**, the default **Cut Option**. UniSim Design calculated the Blend based on the following default values for the boiling point ranges and number of cuts per range:

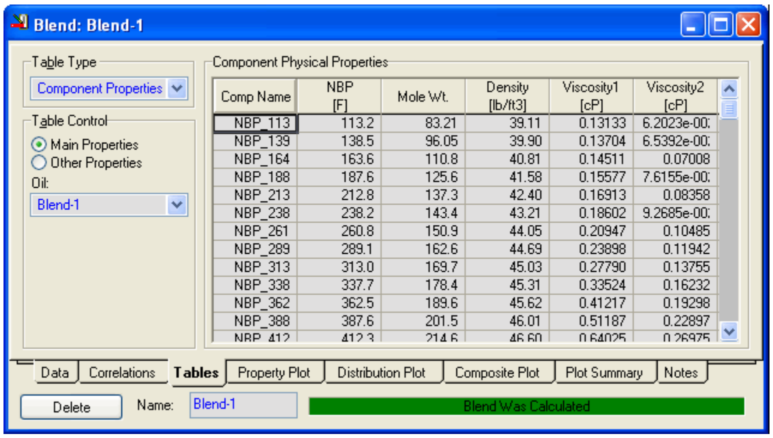
   - IBP to 800°F: 25°F per cut, generating [(800-IBP)/25] hypocomponents
   - 800 to 1200°F: 50°F per cut, generating 8 hypocomponents
   - 1200 to 1400°F: 100°F per cut, generating 2 hypocomponents

   The IBP, or initial boiling point, is the starting point for the first temperature range. The IBP is the normal boiling point (NBP) of the heaviest component in the Light Ends, in this case n-Pentane at

96.9°F. The first range results in the generation of (800-96.9)/25 = 28 hypocomponents. All the cut ranges together result in a total of 28+8+2 = 38 hypocomponents.

5. Click the **Tables** tab to view the calculated properties of these hypocomponents.

Figure 2.30



These components could be used in the simulation. Suppose, however, that you do not want to use the IBP as the starting point for the first temperature range. You could specify another starting point by changing the Cut Option to **User Ranges.** For illustration purposes, 100°F is used as the initial cut point.

6. Return to the **Data** tab.

7. From the Cut Option Selection drop-down list, select User Ranges. The Ranges Selection group appears.

Since the NBP of the heaviest Light Ends component is the starting point for the cut ranges, these hypocomponents were generated on a "light-ends-free" basis. That is, the Light Ends are calculated separately and are not included in these hypocomponents.

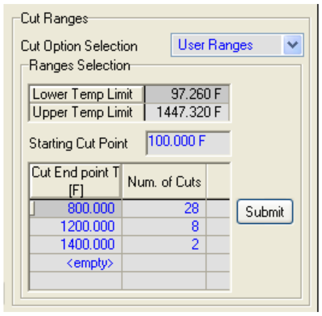
8. In the **Starting Cut Point** field, enter 100°F. This is the starting point for the first range. The same values as the UniSim Design defaults are used for the other temperature ranges.

9. In the Cut End point T column in the table, click on the top cell labeled <**empty**>. The value you will enter in this cell is the upper cut point temperature for the first range (and the lower cut point for the second range).

10. Type **800** then press **ENTER**.

11. Enter the remaining cut point temperatures and the number of cuts values as shown in the figure below.

Figure 2.31

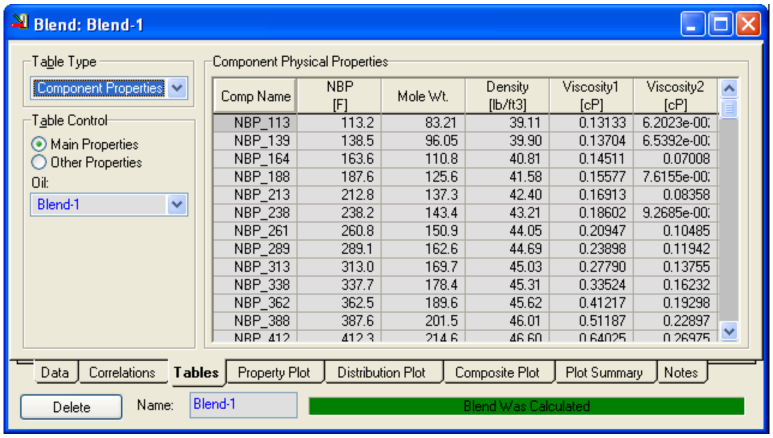


12. Once you have entered the data, click the **Submit** button to calculate the Blend based on the current initial cut point and range values. The message Blend Was Calculated appears in the status bar.

UniSim Design has provided the Initial Boiling Point (IBP) and Final Boiling Point (FBP). The IBP is the normal boiling point (NBP) of the heaviest component in the Light Ends (in this case, n-Pentane). The FBP is calculated by extrapolating the TBP Assay data to 100% distilled.

13. Click the **Tables** tab to view the properties of the petroleum hypocomponents.

Figure 2.32



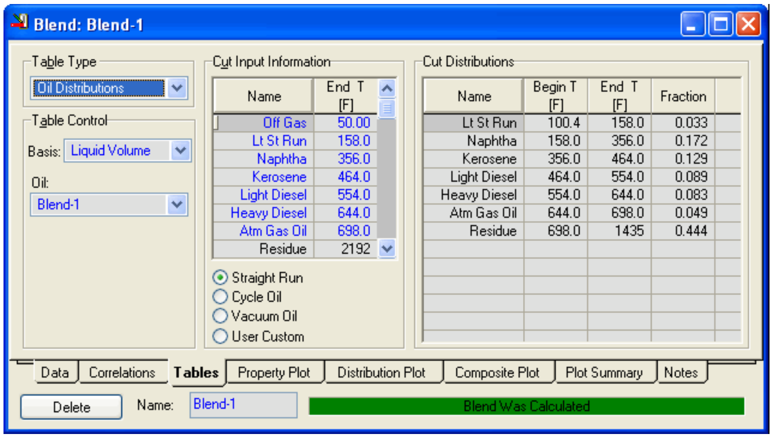
Use the vertical scroll bar to view the components which are not currently visible in the **Component Physical Properties** table.

Viewing the Oil Distributions

1. To view the distribution data, select Oil Distributions from the Table

Type drop-down list. The **Tables** tab is modified as shown below.

Figure 2.33



At the bottom of the Cut Input Information group, the Straight Run radio button is selected, and UniSim Design provides default TBP cut point temperatures for each Straight Run product. The Cut Distributions table shows the Fraction of each product in the Blend. Since Liquid Vol is the current Basis in the Table Control group, the products are listed according to liquid volume fraction.

These fractions can be used to estimate the product flow rates for the fractionation column. For example, the **Kerosene** liquid volume fraction is 0.129. With 100,000 bbl/day of crude feeding the tower, the Kerosene production is expected at **100,000 * 0.129=12,900** or roughly 13,000 bbl/day.

If you want, you can investigate other reporting and plotting options by selecting another **Table Type** or by viewing information on the other tabs in the **Blend** property view.

2. When you are finished, close the **Blend** view to return to the **Oil Characterization** view. Now that the Blend has been calculated, the next task is to install the oil.

Installing the Oil

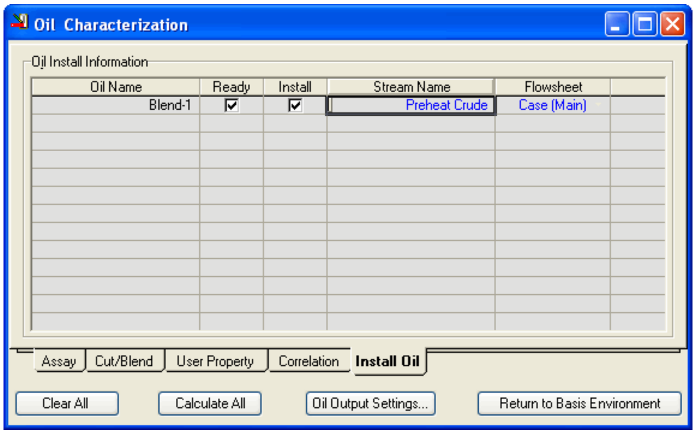
The last step in the oil characterization procedure is to install the oil, which accomplishes the following:

- The petroleum hypocomponents are added to the fluid package.
- The calculated Light Ends and Oil composition are transferred to a material stream for use in the simulation.

1. On the **Oil Characterization** view, click the **Install Oil** tab.
2. In the Stream Name column, click in the top blank cell.

3. Type the name Preheat Crude, then press the **ENTER** key. UniSim Design creates a new stream named Preheat Crude in the flowsheet associated with the fluid package associated with this oil.

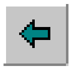
Figure 2.34



In this case, there is only one fluid package (Basis-1) and one flowsheet (the main flowsheet), so the stream is created in the main flowsheet. UniSim Design assigns the composition of the calculated oil and light ends to stream Preheat Crude. The properties of the new stream can be viewed from the Simulation environment.

The characterization procedure is now complete.

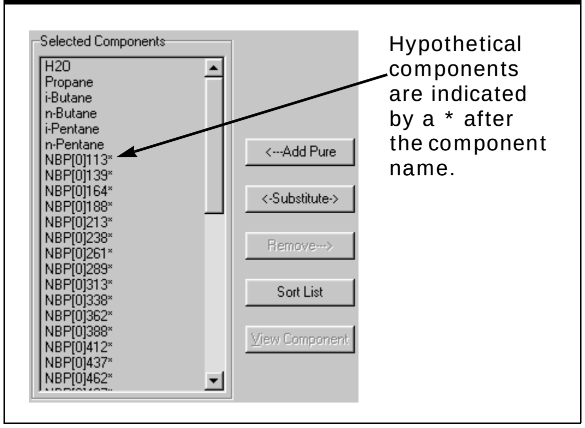
4. Return to the Basis environment by clicking the **Return to Basis Environment** icon.
5. Click the **Components** tab of the Simulation Basis Manager view.
6. Select Component List - 1 from the list in the Component Lists group. Click the **View** button to open the component list property view.



Leave Oil Environment icon

7. The hypocomponents generated during the oil characterization procedure now appear in the Selected Components group.

Figure 2.35



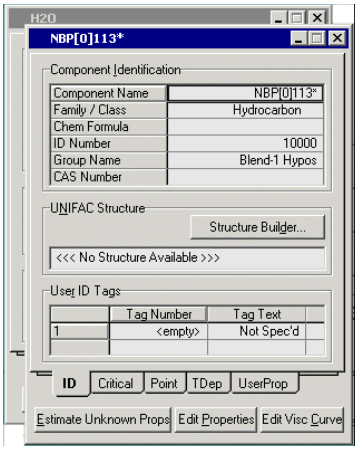
Viewing Component Properties

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

Press and hold the **CTRL** key to select more than one component.

1. In the Selected Components list, select **H2O and NBP[0]113***.
2. Click the **View Component** button. The property views for these two components appear.

Figure 2.36



See **Chapter 3 - Hypotheticals** in the **UniSim Design Simulation Basis Guide** for more information on cloning library components.

The Component property view provides you with complete access to the component information. For pure components like H2O, the information is provided for viewing only. You cannot modify any parameters for a library (pure) component, however, UniSim Design

allows you to clone a library component into a Hypothetical component, which you can then modify as required.

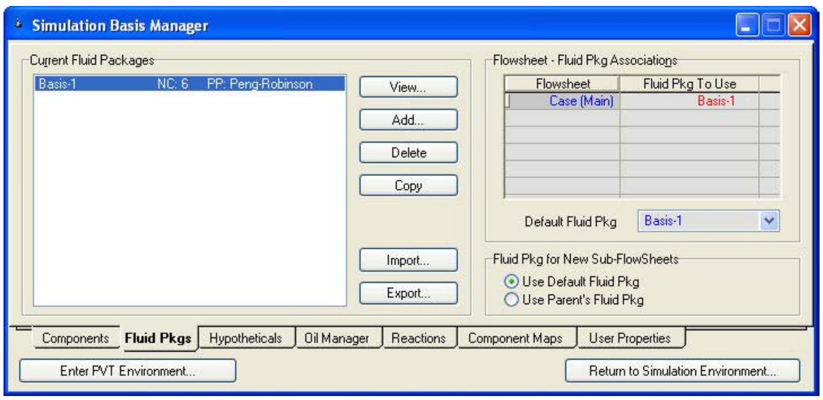
The petroleum hypocomponent shown here is an example of a hypothetical component. You can modify any of the parameters listed for this component. For this example, the properties of the hypothetical components generated during the oil characterization are not changed.

3. Close each of these two component property views.

Basis Manager icon

4. The fluid package is now completely defined, so close the Component List view. The Simulation Basis Manager view should again be visible; if not, click the **Basis Manager** icon to access it.
5. Click the **Fluid Pkgs** tab to view a summary of the new fluid package.

Figure 2.37



The list of Current Fluid Packages displays the new fluid package, Basis-1, showing the number of components (NC) and property package (PP). The fluid package contains a total of 44 components:

- 6 library (pure) components (H2O plus five Light Ends components)
- 38 petroleum hypocomponents

The new fluid package is assigned by default to the Main Flowsheet, as shown in the **Flowsheet-Fluid Pkg Associations** group. Next you will install streams and operations in the Main Simulation environment.

2.2.4 Entering the Simulation Environment

Enter Simulation Environment icon

1. To leave the Basis environment and enter the Simulation

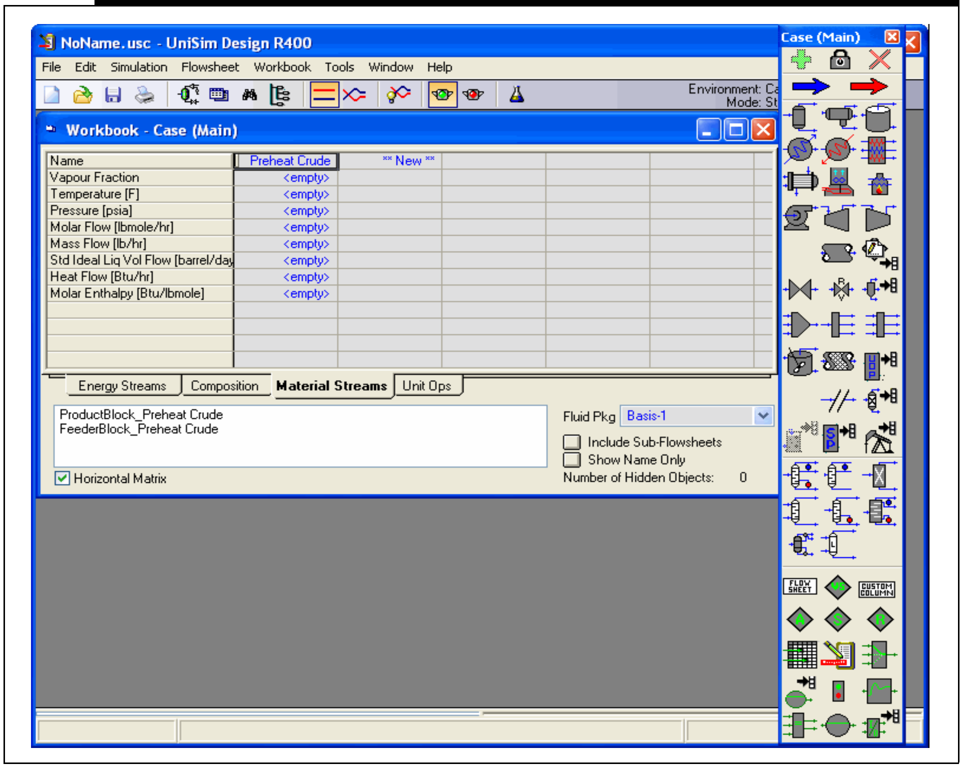
environment, do **one** of the following:

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

When you enter the Simulation Environment, the initial view that appears depends on your current preference setting for the Initial Build Home View.

Three initial views are available: **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 appears. For this example, open the **Workbook** under the **Tools menu** or by pressing **CTRL W**.

Figure 2.38



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 latter two objects

are described below.

Objects	Description
Workbook	A multiple-tab view containing information regarding 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 which can be used to add streams and unit operations.

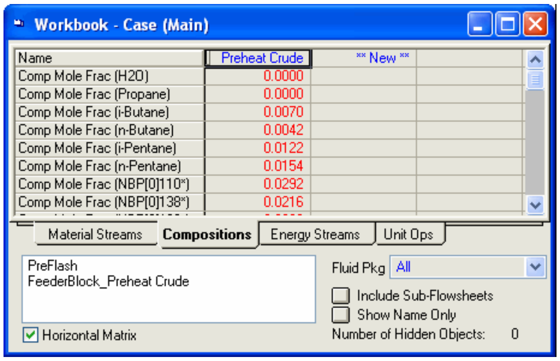
You can toggle the palette open or closed by pressing **F4**, or by selecting Open/Close Object Palette from the Flowsheet menu.

Also notice that the name of the stream (Preheat Crude) you created during the Oil characterization procedure appears in the Workbook, and the white Object Status window at the very bottom of the environment view shows that the stream has an unknown pressure. As you specify the conditions of Preheat Crude, the message displayed in the Object Status window is updated appropriately. Before specifying the feed conditions, you can view the stream composition, which was calculated by the Oil characterization.

Viewing the Feed Composition

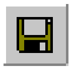
1. In the Workbook, click the **Compositions** tab to view the composition of the streams.

Figure 2.39



The Light Ends and petroleum hypocomponents are listed by Mole Fraction. To view the components which are not currently visible, use the up and down arrow keys or the vertical scroll bar to advance down the component list.

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



Save icon

2. Do one of the following:
   - Click the **Save** icon on the toolbar.

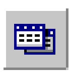
- Select **Save** from the **File** menu.
- Press **CTRL S**.

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 UniSim Design directory.

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

3. In the **File name** field, type a name for the case, for example REFINING. You do not have to enter the *.usc extension; UniSim Design adds it automatically.
4. Once you have entered a file name, press the **ENTER** key and UniSim Design saves the case under the name you gave it. The Save As view does not appear again unless you choose to give it a new name using the **Save As** command.

2.2.5 Using the Workbook



Workbook icon

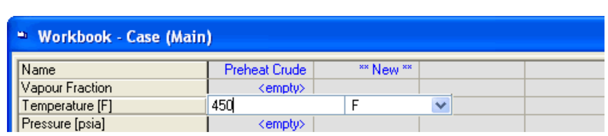
Click the Workbook icon on the toolbar to ensure the **Workbook view** is active.

Specifying the Feed Conditions

In general, the first task in the Simulation environment is to install one or more feed streams, however, the stream Preheat Crude was already installed during the oil characterization procedure. At this point, your current location should be the **Compositions** tab of the **Workbook** view.

1. Click the **Material Streams** tab. The preheated crude enters the pre-fractionation train at 450°F and 75 psia.
2. In the Preheat Crude stream, click in the **Temperature** cell and type 450. UniSim Design displays the default units for temperature, in this case °F.

Figure 2.40



When you press **ENTER** after entering a stream property, you are advanced down one cell in the Workbook only if the cell below is <empty>. Otherwise, the active cell remains in its current location.

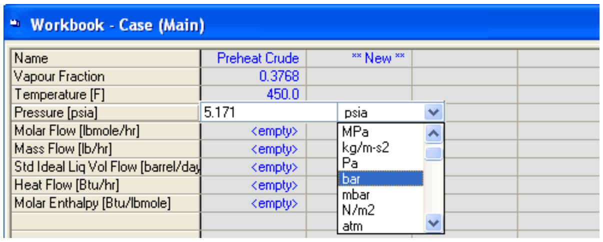
3. Since this is the correct unit, press the **ENTER** key. UniSim Design accepts the temperature. UniSim Design advances to the **Pressure** cell.

   If you know the stream pressure in another unit besides the default of psia, UniSim Design will accept your input in any one of a number of different units and automatically convert the value to the default. For example, the pressure of Preheat Crude is 5.171 bar, but the

default units are psia.

4. In the **Pressure** cell, type 5.171.
5. Press **SPACE BAR**. The field containing the active cell units becomes active.
6. Begin typing 'bar'. The field opens a drop-down list and scrolls to the unit(s) most closely matching your input.

Figure 2.41



Alternately, you can specify the unit simply by selecting the unit in the drop-down list.

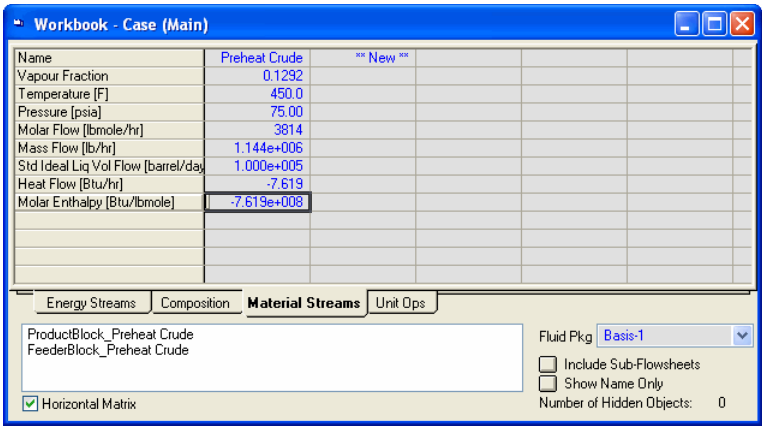
7. Once 'bar' is selected, press the **ENTER** key. UniSim Design accepts the pressure and automatically converts to the default unit, psia.
8. Click in the **Liquid Volume Flow** cell, then type 1e5. The stream flow is entered on a volumetric basis, in this case 100,000 barrel/day.
9. Press the **ENTER** key.

If UniSim Design does not flash the stream, ensure that the Solver Active icon in the tool bar is selected.

Solver Active icon

The stream is now completely defined, so UniSim Design flashes it at the conditions given to determine the remaining properties. The properties of Preheat Crude are shown below. The values you specified are a different colour (blue) than the calculated values (black).

Figure 2.42



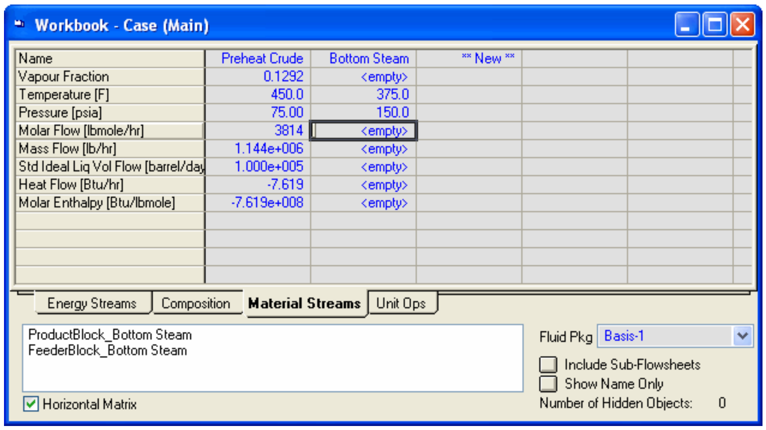
The next task is to install and define the utility steam streams that will be attached to the fractionation tower later.

Installing the Utility Steam Streams

1. On the **Material Streams** tab, click in the header cell labeled ****New****.
2. Type the new stream name Bottom Steam, then press **ENTER**. UniSim Design creates the new stream.
3. In the **Temperature** cell, enter 375°F.
4. In the **Pressure** cell, enter 150 psia.

UniSim Design accepts blank spaces within a stream or operation name.

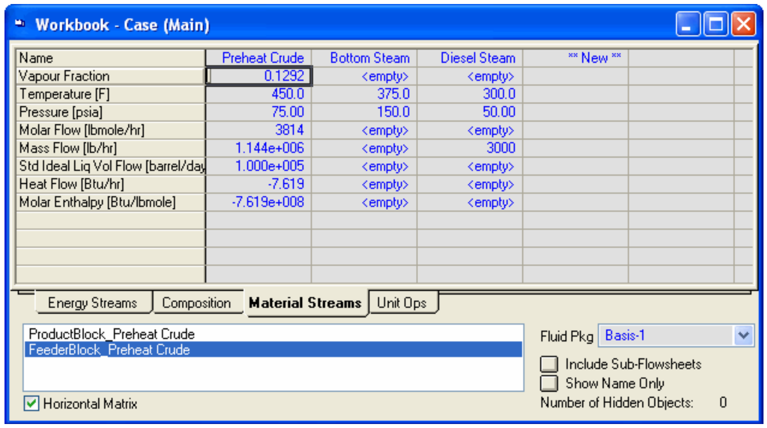
Figure 2.43



5. In the **Mass Flow** cell, enter 7500 lb/hr.
6. Create a new utility stream called Diesel Steam.
7. Define the conditions of this stream as follows:
   - Temperature 300°F
   - Pressure 50 psia
   - Mass Flow 3000 lb/hr.

   The Workbook view appears as shown below.

Figure 2.44



Providing Compositional Input

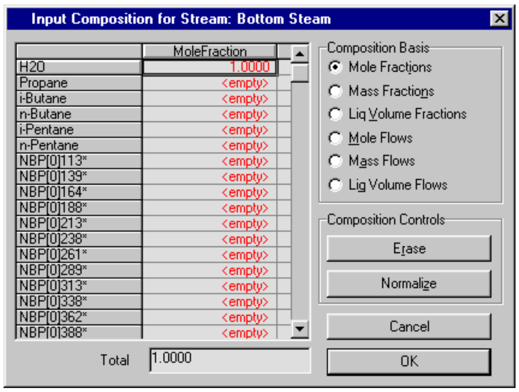
Now that the utility stream conditions have been specified, the next task is to input the compositions.

1. Click the **Compositions** tab in the Workbook. The components are listed by Mole Fraction by default.
2. In the Bottom Steam column, click in the input cell for the first component, H2O.
3. Since the stream is all water, type 1 for the H2O mole fraction, then press **ENTER**.

   The Input Composition for Stream view appears, allowing you to complete the compositional input.

   The Input Composition for Stream view is Modal, indicated by the absence of the Minimize/Maximize icons in the upper right corner.

Figure 2.45



When a Modal view is visible, you are unable to move outside the view until you are finish with it, by clicking either the Cancel or OK button.

The Input Composition for Stream view allows you to specify a stream composition quickly and easily. The following table lists and

describes the features available on this view:

These are the default colours; yours can appear differently depending on your settings on the Colours page of the Session Preferences 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 (2 parts N2, 2 parts CO2, etc.) Rather than manually converting these ratios to fractions summing to one, enter the numbers of parts for each component and click the Normalize button. UniSim Design 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, enter the fractions (or the actual flows) for the non-zero components, leaving the others <empty>. Click the Normalize button, and UniSim Design 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 composition has been 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, then click the OK button. • Input the fractions (totalling 1.000), flows or relative number of parts of all non-zero components, then click the Normalize button then the OK button. • Input the flows or relative number of parts of all components, including any zero components, then click the OK button.

This stream is pure water, therefore, there is no need to enter fractions for any other components.

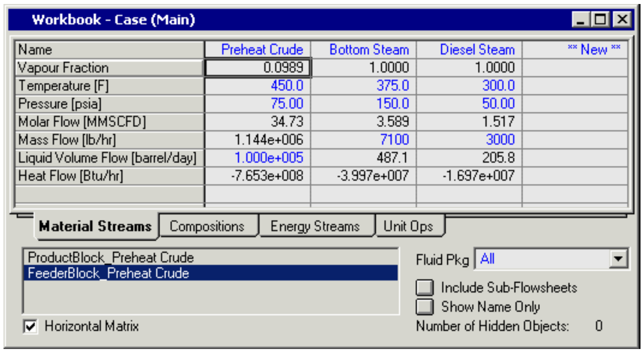
4. Click the **Normalize** button and all other component fractions are forced to zero.
5. Click the **OK** button. UniSim Design accepts the composition and you are returned to the Workbook view.

   The stream is now completely defined, so UniSim Design flashes it at the conditions given to determine the remaining properties.
6. Repeat steps #2 to #5 for the other utility stream, Diesel Steam.

If you want to delete a stream, move to the Name cell for the stream, then press **DELETE**. UniSim Design ask for confirmation of your action.

7. Click the **Material Streams** tab. The calculated properties of the two utility streams appear here.

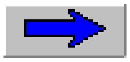
Figure 2.46



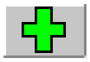
Next, you will learn alternative methods for creating a new stream.

8. To add the third utility 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 on the Palette's **Add Object** icon.

   Each of these four methods displays the property view for the new stream, which is named according to the **Auto Naming** setting in your **Preferences**. The default setting names new material streams with numbers, starting at 1, and energy streams starting at **Q-100**.



Material Stream icon



Add Object icon

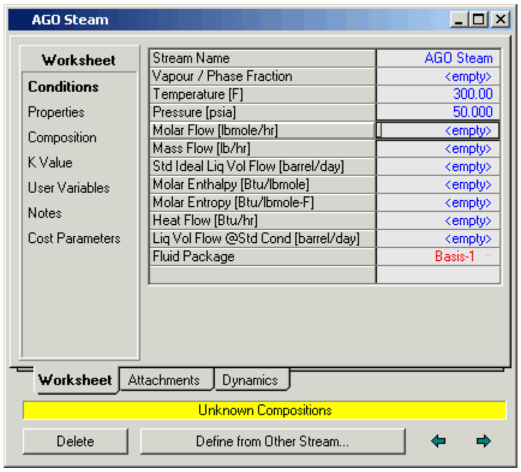
9. In the stream property view, click in the **Stream Name** cell and rename the stream **AGO Steam**.
10. Press **enter**.
11. In the **Temperature** cell, enter **300.**

Both of the temperature and pressure parameters are in the default units, so you do not need to change the unit with the values.

Do not enter a flow, it is entered through the **Composition** page.

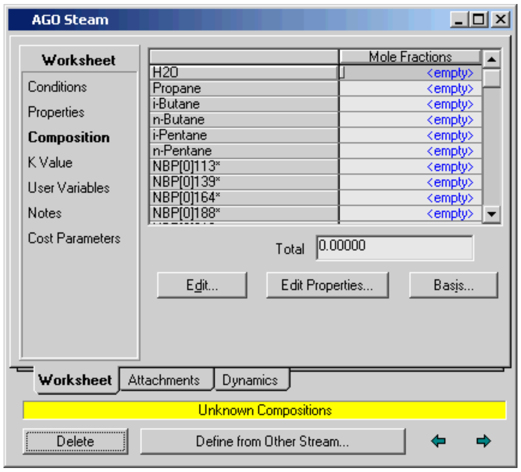
12. In the **Pressure** cell, enter **50**.

Figure 2.47



13. Select the **Composition** page to begin the compositional input for the new stream.

Figure 2.48



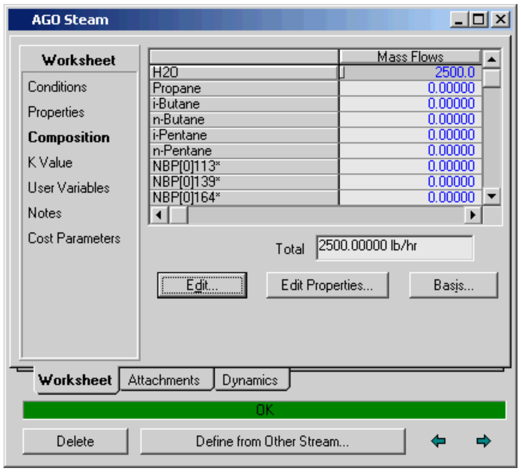
The current Composition Basis setting is set to the Preferences Default of Mole Fractions. The stream composition is entered on a mass basis.

14. Click the **Edit** button. The Input Composition for Stream view appears.
15. In the Composition Basis group, select the **Mass Flows** radio button.
16. Click in the compositional cell for H2O.
17. Type 2500 for the steam mass flow, then press **ENTER**. As there are no other components in this stream, the compositional input is complete.

Since only H2O contain any significant value, UniSim Design automatically forces all other components' value to be zero.

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

Figure 2.49



UniSim Design performs a flash calculation to determine the unknown properties of AGO Steam, as shown by the status indicator displaying 'OK'. You can view the properties of each phase using the horizontal scroll bar in the matrix or by re-sizing the property view. In this case, the stream is superheated vapour, so no Liquid phase exists and the Vapour phase is identical to the overall phase. To view the vapour compositions for AGO Steam, scroll to the right by clicking the right scroll arrow, or by click and dragging the scroll button.

The compositions are currently displayed by Mass Flows. You can change this by clicking the Basis button and choosing another Composition Basis radio button.

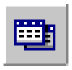
19. Close the AGO Steam property view.

2.2.6 Installing Unit Operations

Now that the feed and utility streams are known, the next task is to install the necessary unit operations for processing the crude oil.

Installing the Separator

The first operation is a Separator, used to split the feed stream into its liquid and vapour phases. As with most commands in UniSim Design, installing an operation can be accomplished in a number of ways. One

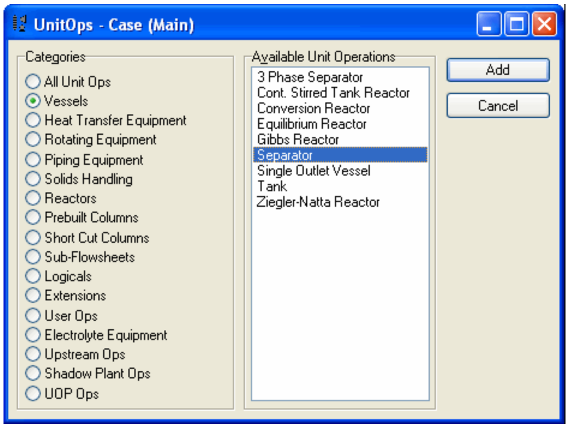


Workbook icon

method is through the Unit Ops tab of the Workbook.

1. Click the **Workbook** icon to ensure the Workbook is the active view.
2. Move to the **Unit Ops** tab.
3. Click the **Add UnitOp** button. The UnitOps view appears, listing all available unit operations.
4. In the Categories group, select the **Vessels** radio button. UniSim Design produces a filtered list of unit operations, showing only those in the current category.

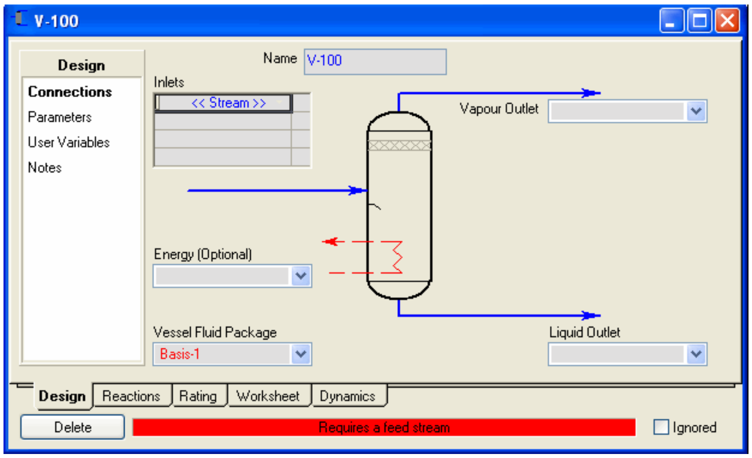
Figure 2.50



5. Add the separator by doing **one** of the following:
   - Select Separator in the list of Available Unit Operations, and click the **Add** button or the **ENTER** key.
   - Double-click on Separator.

   The property view for the **separator** appears in the figure below.

Figure 2.51



UniSim Design provides the default name **V-100** for the **separator**. The default naming scheme for unit operations can be changed in your Session Preferences.

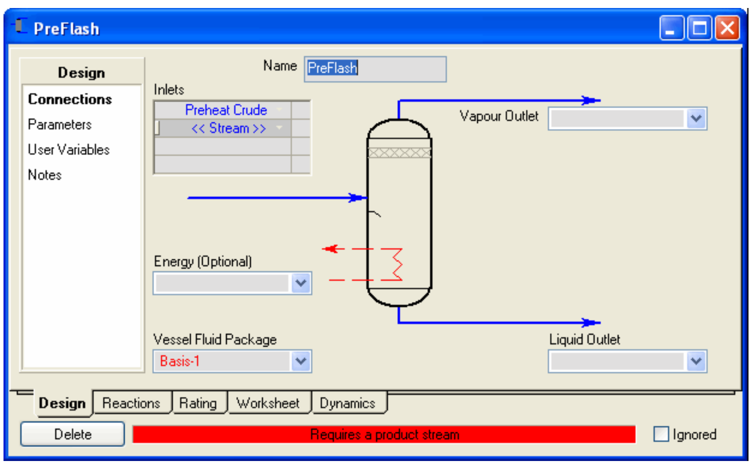
A unit operation property view contains all the information defining the operation, organized into tabs and pages. The Design, Rating, and Worksheet tabs appear for most operations. Property views for more complex operations contain more tabs.

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

6. Click in the **Name** field, type **PreFlash**, then press **enter**. The status indicator at the bottom of the view shows that the operation requires a feed stream.
7. In the Inlets matrix, click in the <**<Stream>**> cell.
8. Click the down arrow to open the drop-down list of available streams.
9. Select **Preheat Crude** from the list. Preheat Crude appears in the Inlets matrix, and the <**<Stream>**> label is automatically moved down to a new empty cell. The status indicator now displays '**Requires a product stream'**.

Alternatively, you could have made the connection by typing the exact stream name in the cell, and pressing **ENTER**.

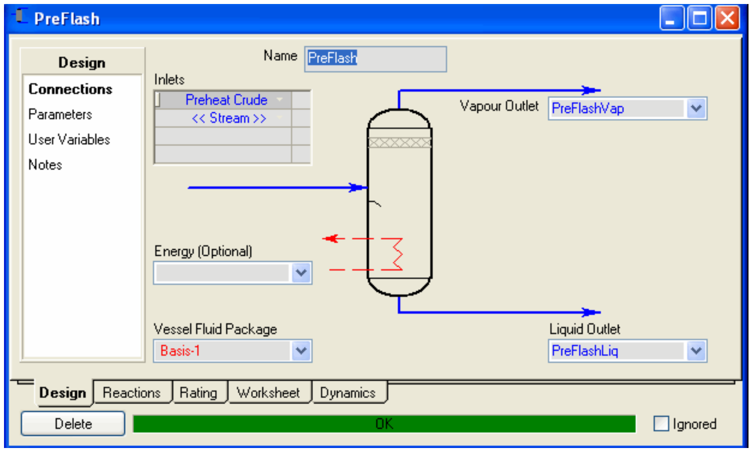
Figure 2.52



10. Click in the **Vapour Outlet** field, or press **tab** to move to the field.
11. Type **PreFlashVap** in the field, then press **enter**. This stream does not yet exist, so UniSim Design creates this new stream.

12. Click in the **Liquid Outlet** field and type **PreFlashLiq**. UniSim Design creates another new stream**.**

Figure 2.53

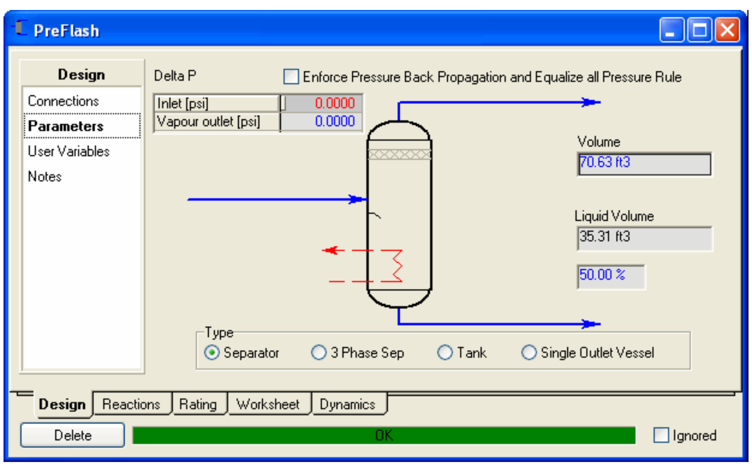


An **Energy** stream could be attached to heat or cool the vessel contents, however, for the purposes of this example, the energy stream is not required.

The status indicator displays a green **OK message**, showing that the operation and attached streams are completely calculated.

13. Select the **Parameters** page. The default **Delta P** (pressure drop) of zero is acceptable for this example. The **Liquid Level** is also acceptable at its default value.

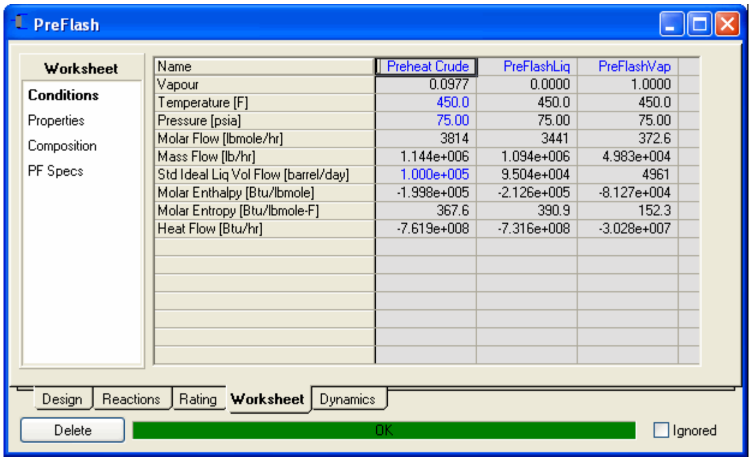
Figure 2.54



Since there is no energy stream attached to the **separator**, no **Optional Heat Transfer** information is required.

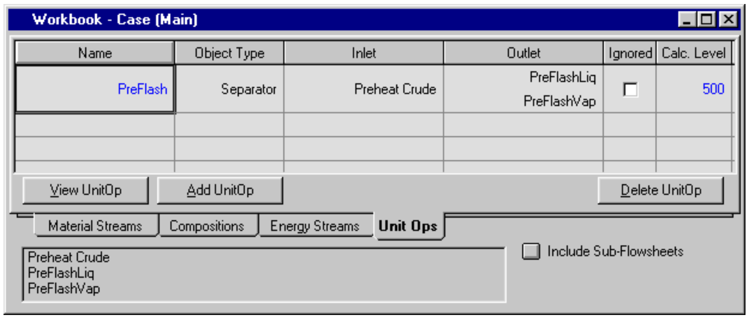
14. To view the calculated outlet streams, click the **Worksheet** tab. This is a condensed Workbook displaying only those streams attached to the operation.

Figure 2.55



15. Now that the **separator** is completely known, close the PreFlash view and the UnitOps view, and return to the **Workbook view**. The new separator appears on the **Unit Ops** tab.

Figure 2.56



The matrix shows the operation **Name**, its **Object Type**, the attached streams (**Inlet** and **Outlet**), whether it is **Ignored**, and its **Calculation Level**.

Optional Methods for Accessing Property Views

When you click the View UnitOp button, the property view for the operation occupying the active row in the matrix opens. Alternatively, by double-clicking on any cell (except **Inlet** and **Outlet**) associated with the operation, you also open its property view.

You can also open the property view for a stream directly from the Unit Ops tab of the Workbook. When any of the **Name**, **Object Type**, **Ignored** or **Calc**. Level cells are active, the display field at the bottom of the view displays all streams attached to the current operation. Currently, the **Name** cell for **PreFlash** is active, and the display field displays the three streams attached to this operation. To open the property view for one of the streams attached to the **separator** (such as **Preheat Crude)**, do **one** of the following:

- Double-click on Preheat Crude in the display field at the bottom of the view.
- Double-click on the **Inlet** cell for PreFlash. The property view for the first listed feed stream opens. In this case, Preheat Crude is the only feed stream, so its property view also opens.

2.2.7 Using Workbook Features

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

Accessing Unit Operations from the Workbook

Return to the Material Streams tab of the Workbook.

Any utilities attached to the stream with the Workbook active are also displayed in (and are accessible through) this display field.

There are a number of ways to open the property view for an operation directly from the **Workbook** besides using the **Unit Ops** tab.

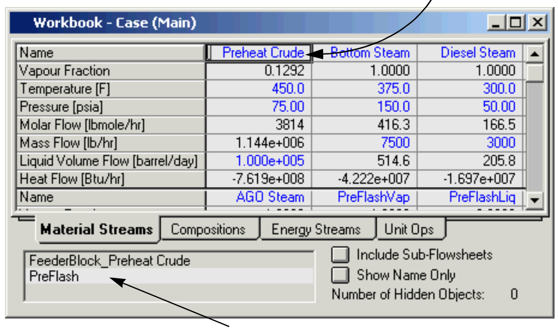
When your current location is a Workbook streams tab (Material Streams, Compositions, and Energy Streams tabs), the field at the bottom of the Workbook view displays the operations to which the current stream is attached. In this display field, you can click on any cell associated with the stream.

For example, if you click in any cell for Preheat Crude, the field displays the name of the operation, PreFlash, to which this stream is attached. The display field also displays FeederBlock_Preheat Crude, because the Preheat Crude stream is a boundary stream. To access the property view for the PreFlash operation, double-click on PreFlash. The operation

property view appears.

Figure 2.57

Stream Preheat Crude is the current Workbook location.



The operation to which Preheat Crude is attached appears in this display field. Double-click the operation name to access its property view.

Adding a Tab to the Workbook

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

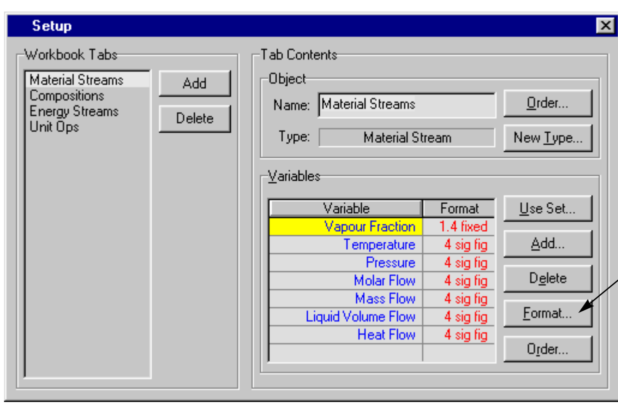
In this section, you will create a new Workbook tab that displays only stream pressure, temperature, and flow.

1. Do one of the following:
   - From the **Workbook** menu, 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.

The four existing tabs are listed in the **Workbook Tabs** area. When you add a new tab, it is inserted *before* the selected tab (currently **Material Streams**). You will insert the new tab before the **Compositions** tab.

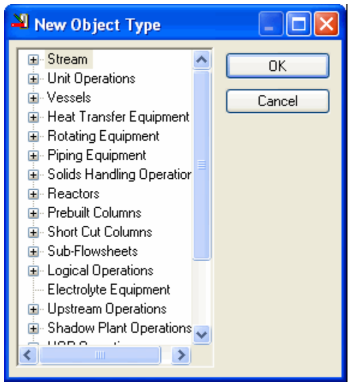
Figure 2.58



Currently, all variables appear with four significant figures. You can change the display format or precision of any Workbook variables by clicking the Format button.

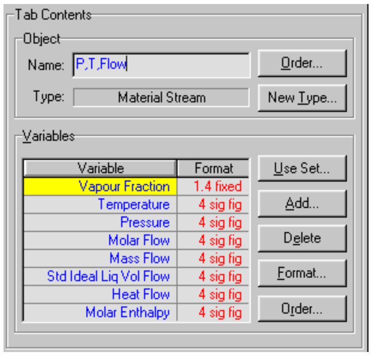
2. In the Workbook Tabs group list, select **Compositions**.
3. Click the **Add** button. The **New Object Type** view appears.

Figure 2.59



4. Click the **+** beside Stream, select **Material Stream** from the branch, then click the **OK** button. You return to the **Setup** view, and the new tab appears after the existing **Material Streams** tab.
5. In the Tab Contents Object group, click in the **Name** field.
6. Change the name of the new tab to **P,T,Flow** to better describe the tab contents.

Figure 2.60



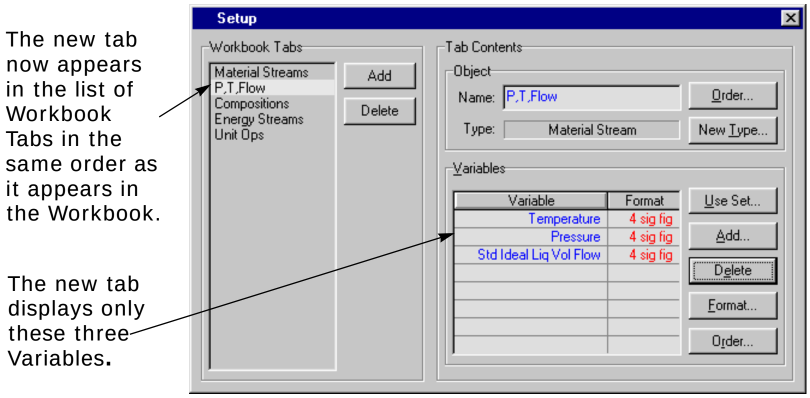
The next task is to customize the tab by removing the variables that are not required.

7. In the Variables group, click on the first variable, **Vapour Fraction**.
8. Press and hold the **CTRL** key.
9. Click on the other variables, **Molar Flow**, **Mass Flow**, **Heat Flow,** and Molar Enthalpy. These four variables are now highlighted.
10. Release the **ctrl** key.

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

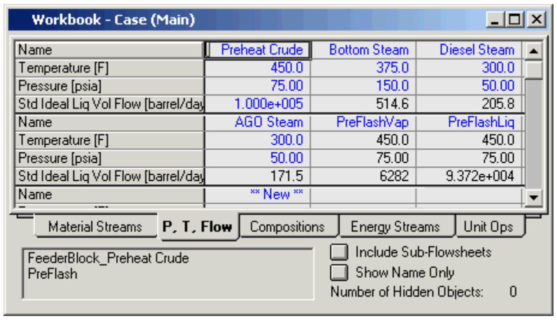
11. Click the **Delete** button to remove them from this **Workbook** tab. The finished **Setup** view appears below.

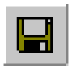
Figure 2.61



12. Click the **Close** icon to return to the **Workbook** view and see the new tab.

Figure 2.62

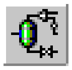




Save icon

13. Save your case by doing **one** of the following:
   - Click the **Save** icon on the tool bar.
   - Select **Save** from the **File** menu.
   - Press **CTRL S**.

2.2.8 Using the PFD



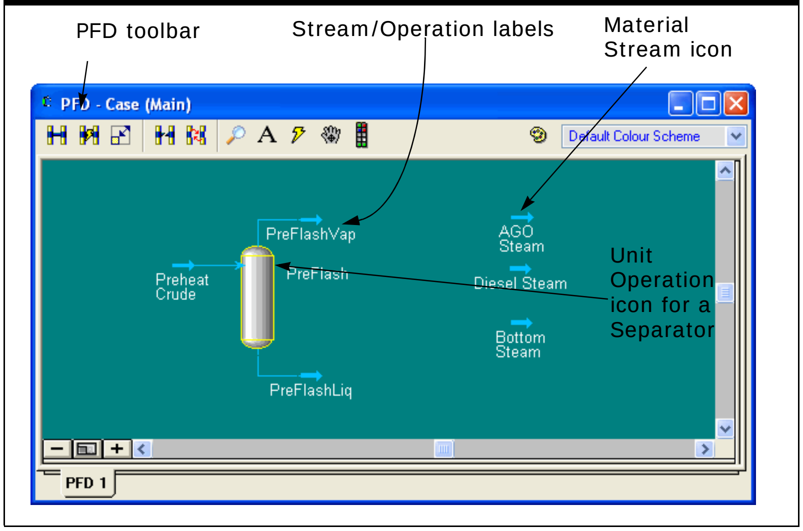
PFD icon

The **PFD** is the other main view used in UniSim Design. The **PFD** item appears in the UniSim Design menu bar whenever the **PFD** is active.

1. To open the **PFD**, click the **PFD** icon on the tool bar. The **PFD** view should appear similar to the one shown below, except some stream

icons may overlap each other.

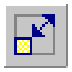
Figure 2.63



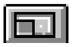
As a graphical representation of your flowsheet, the **PFD** shows the connections among all streams and operations, also known as ‘objects’. Each object is represented by a symbol, also known as an ‘icon’. A stream icon is an arrow pointing in the direction of the flow, while an operation icon is a 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 three utility stream icons below and to the left of the **Separator**. To move an icon, click and drag it to the new location.

You can click and drag either the icon (arrow) itself, or the label (stream name), as these two items are grouped together.


Size Mode icon


Zoom Out 25% icon


Display Entire PFD icon


Zoom In 25% icon

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

Other things you can do while the **PFD** is active include the following:

- Access commands and features through the **PFD** toolbar.
- Open the property view for an object by double-clicking on its icon.
- Move an object by click and dragging it to the new location.
- Access “pop-up” summary information for an object simply by placing the cursor over it.
- Change an icon's size by clicking the Size Mode icon, clicking on the icon, and click and dragging the sizing handles that appear around the icon.

- 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 corner of the PFD view.

Some of these functions are illustrated here; for more information, see **Section 7.25 - PFD** in the **UniSim Design User Guide**.

Calculation Status

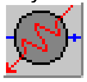
Before proceeding, you will examine a feature of the PFD that allows you to trace the calculation status of the objects in your flowsheet. If you recall, the status indicator at the bottom of the property view for a stream or operation displays one of three possible states for the object:

Keep in mind that these are the UniSim Design default colours; you can change the colours in the Session Preferences.

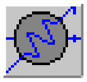
Status	Description
Red Status	A major piece of defining information is missing from the object. For example, a feed or product stream is not attached to a separator. The status indicator is red, and an appropriate warning message appears.
Yellow Status	All major defining information is present, but the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

When you are in the **PFD**, the streams and operations are colour-coded to indicate their calculation status. The inlet separator is completely calculated, so its normal colours appear. While installing the remaining operations through the **PFD**, their colours (and status) changes appropriately as information is supplied.

The icons for all streams installed to this point are dark blue, indicating they have been flashed.



Heater icon (Red)



Cooler icon (Blue)

A similar 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 Crude Furnace

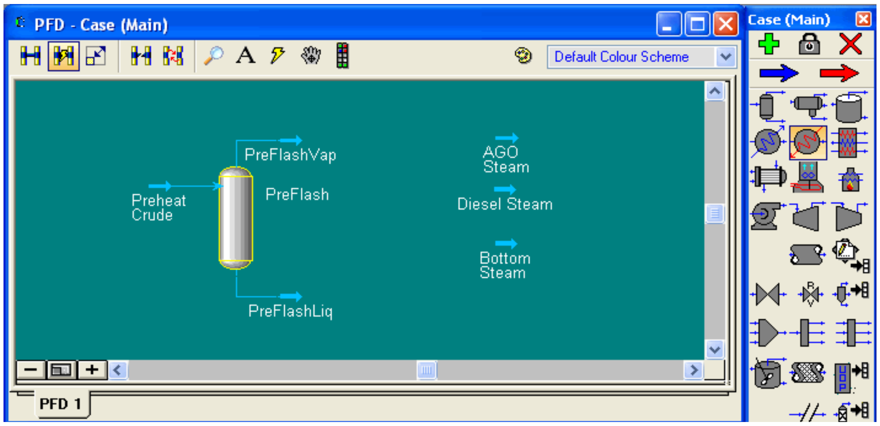
In this section, you will install a crude furnace. The furnace is modeled as a **Heater**.

1. Ensure the **Object Palette** is visible (if it is not, press **F4)**.

   You will add the furnace to the right of the PreFlash Separator, so make some empty space available by scrolling to the right using the horizontal scroll bar.

2. In the Object Palette, click the **Heater** icon. The cursor changes to a special cursor, with a black frame and plus (+) symbol attached to it. The frame indicates the size and location of the operation icon.
3. Position the cursor over the **PFD** to the right of the **separator**.

Figure 2.64



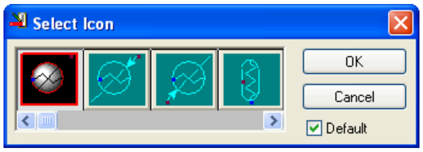
Notice the **heater** has red status (colour), indicating that it requires feed and product streams.

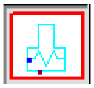
4. Click to ‘drop’ the **heater** onto the **PFD**. UniSim Design creates a new **heater** with a default name, **E-100**.

   Next you will change the **heater** icon from its default to one more closely resembling a furnace.

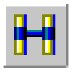
5. Right-click the **heater** icon. The Object Inspect menu appears.
6. Select **Change Icon** from the menu. The **Select Icon** view appears.

Figure 2.65





Furnace icon



Attach Mode icon

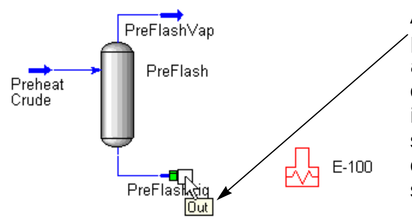
7. Click the **WireFrameHeater5** icon (scroll to the right), then click the **OK** button. The new icon appears in the **PFD**.

Attaching Streams to the Furnace

When you are in **Attach** mode, you are not 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** icon on the PFD tool bar to enter **Attach** mode.
2. Position the cursor over the right end of the **PreFlashLiq** stream icon. A small box appears at the cursor tip.

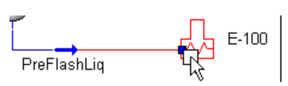
Figure 2.66

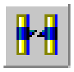


At the square connection point, a pop-up description appears attached to the cursor. The pop-up “Out” indicates which part of the stream is available for connection, in this case, the stream outlet.

3. With the pop-up ‘Out’ visible, click and hold the mouse button. The white box becomes black, indicating that you are beginning a connection.
4. Drag the cursor toward the left (inlet) side of the **heater**. A trailing line appears between the **PreFlashLiq** stream icon and the cursor, and a connection point appears at the **Heater** inlet.
5. Place the cursor near the connection point of the heater, and the trailing line snaps to that point. As well, a white box appears at the cursor tip, indicating an acceptable end point for the connection.

Figure 2.67





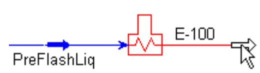
Break Connection icon

If you make an incorrect connection:

1. Click the **Break Connection** icon on the **PFD** toolbar.
2. Move the cursor over the stream line connecting the two icons. A checkmark attached to the cursor appears, indicating an acceptable connection to break.
3. Click once to break the connection.

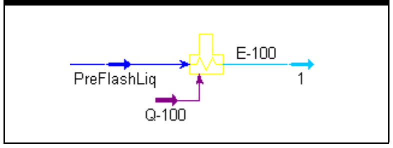
6. Release the mouse button, and the connection is made to the **heater** inlet.
7. Position the cursor over the right end of the **heater** icon. The connection point and pop-up ‘Product’ appears.
8. With the pop-up visible, click and hold the mouse button. The white box again becomes black.
9. Move the cursor to the right of the **heater**. A stream icon appears with a trailing line attached to the **heater** outlet. The stream icon indicates that a new stream is being created.

Figure 2.68



10. With the stream icon visible, release the mouse button. UniSim Design creates a new stream with the default name **1**.
11. Create the **Heater** energy stream, starting the connection from the bottom left connection point on the Heater icon labeled 'Energy Stream'. The new stream is automatically named **Q-100**, and the **heater** now has yellow (warning) status. This status indicates that all necessary connections have been made, but the attached streams are not entirely known.

Figure 2.69



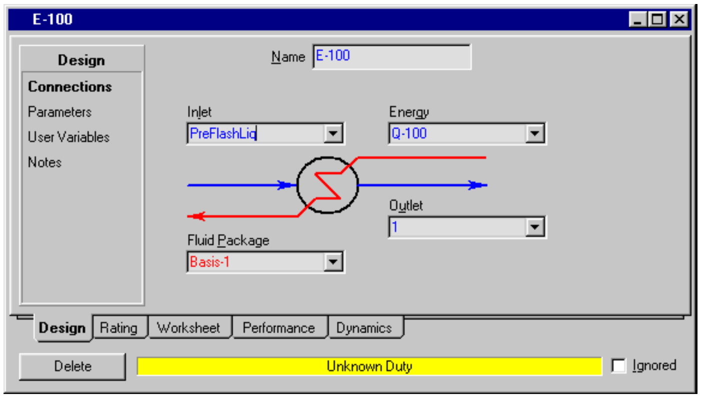
12. Click the **Attach** icon again to return to **Move** mode.

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

Modifying Furnace Properties

1. Double-click the **Heater** icon to open its property view.
2. Click the **Design** tab, then select the **Connections** page. The names of the Inlet, **Outlet,** and **Energy** streams appear in the appropriate fields.

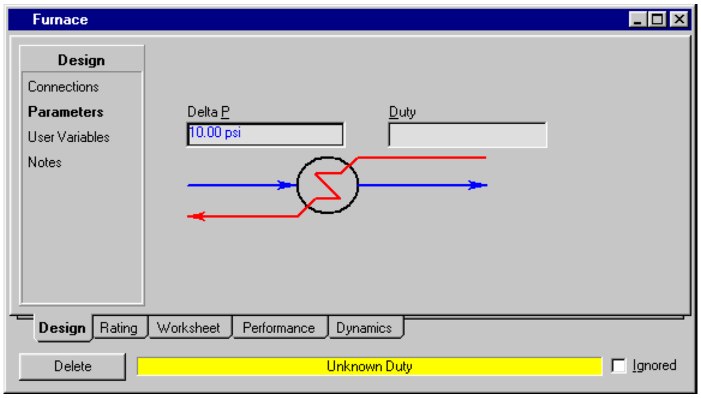
Figure 2.70



3. In the **Name** field, change the operation **name** to **Furnace**.
4. Select the **Parameters** page.

5. In the **Delta P field, enter 10** psi, then close the view.

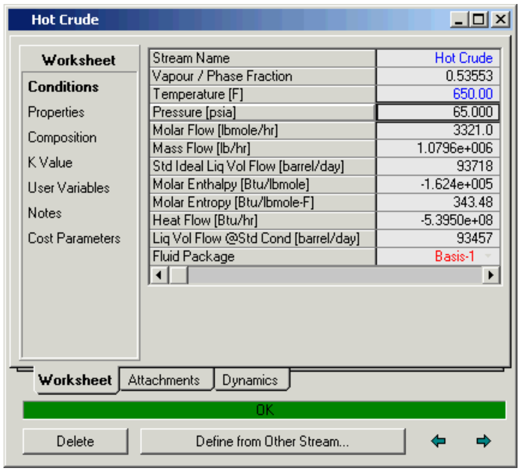
Figure 2.71



The **Furnace** has one available degree of freedom. Either the outlet stream temperature or the amount of duty in the energy stream can be specified. In this case, you will specify the outlet temperature.

6. Double-click the outlet stream icon (**1**) to open its property view.
7. In the **Stream Name** field, change the n**ame** to **Hot Crude**.
8. In the **Temperature** field, specify a temperature of **650**°F.

Figure 2.72

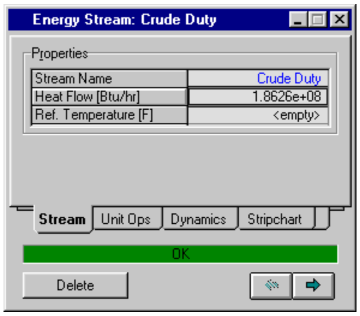


The remaining degree of freedom in the Furnace has now been used, so UniSim Design can flash **Hot Crude** and determine its remaining properties.

9. Close the view to return to the **PFD view**. The **Furnace** now has green status, and all attached streams are known.

10. Double-click on the energy stream icon (**Q-100**) to open its property view. The required heating duty calculated by UniSim Design appears in the **Heat Flow** cell.
11. In the **Stream Name** cell, rename this energy stream **Crude Duty**, then close the property view.

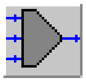
Figure 2.73



Installing the Mixer

In this section, you will install a Mixer operation. The **Mixer** is used to combine the hot crude stream with the vapours bypassing the furnace. The resulting stream is the feed for the crude column.

1. Make some empty space available to the right of the **Furnace** using the horizontal scroll bar. Move other objects if necessary.
2. Click the **Mixer** icon on the **Object Palette**.

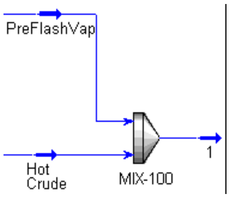


Mixer icon

3. Position the cursor over the **PFD** to the right of the **Hot Crude** stream icon.
4. Click to 'drop' the **mixer** onto the **PFD**. UniSim Design creates a new **mixer** with the default name **MIX-100**.
5. Press and hold the **CTRL** key to temporarily enable the Attach mode while you make the **mixer** connections (you will not release it until step #13).
6. Position the cursor over the right end of the **PreFlashVap** stream icon. The connection point and pop-up 'Out' appears.
7. With the pop-up visible, click and hold the mouse button, then drag the cursor toward the left (inlet) side of the **mixer**. Multiple connection points appear at the **mixer** inlet.

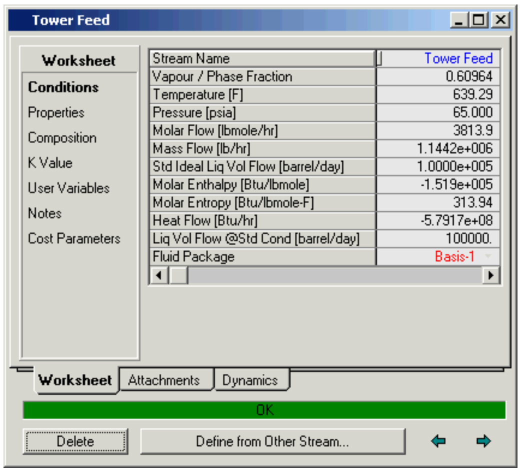
Multiple connection points appear because the **Mixer** accepts multiple feed streams.

8. Place the cursor near the inlet area of the **mixer**, and when the white box appears at the cursor tip, release the mouse button to make the connection.
9. Repeat steps #6 to #8 to connect the **Hot Crude** stream to the **Mixer**.
10. Position the cursor over the right end of the **mixer** icon. The connection point and pop-up 'Product' appears.



11. With the pop-up visible, click and drag to the right of the **mixer**. A white stream icon appears, with a trailing line attached to the **mixer** outlet.
12. With the white stream icon visible, release the mouse button. UniSim Design creates a new stream with the default name **1**.
13. Release the **ctrl** key to leave **Attach** mode.
14. Double-click on the outlet stream icon **1** to access its property view. When you created the **mixer** outlet stream, UniSim Design automatically combined the two inlet streams and flashed the mixture to determine the outlet conditions.
15. In the **Stream Name** cell, rename the stream **Tower Feed**, then close the view.

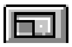
Figure 2.74



16. Double-click the **mixer** icon, **MIX-100**. Change the name to **Mixer**, then close the view.

Resizing Icons in the PFD

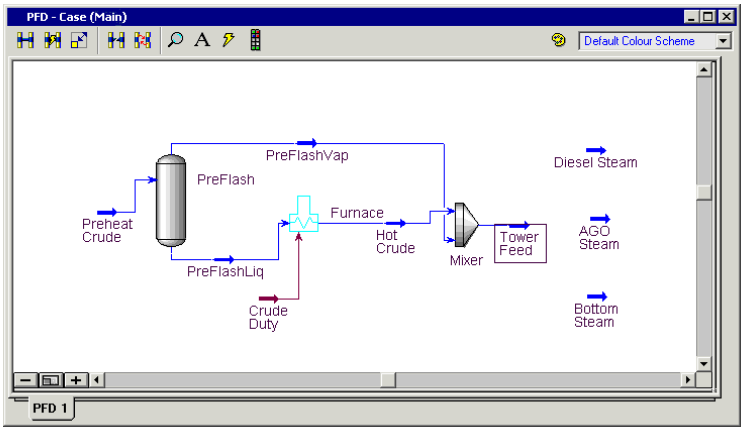
Resize icons in the PFD to make it easier to read.

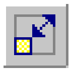


Zoom All icon

1. Resize the PFD view by clicking and dragging the outside border.
2. Click the **Zoom All ic**on to fill the **PFD** window, including any objects that were not visible previously. A possible view of the resized **PFD** appears in the figure below.

Figure 2.75

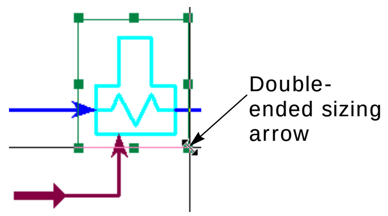




Size Mode icon

3. Click the **Size Mode** icon on the **PFD** toolbar.
4. Click the **Furnace** icon in the **PFD**. A frame with sizing handles appears around the icon.
5. Place the cursor over one of the sizing handles. The cursor changes to a double-ended sizing arrow.

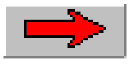
Figure 2.76



6. With the sizing arrow visible, click and drag to resize the icon.
7. Click the **Size Mode** icon again to return to Move mode.

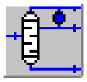
Adding an Energy Stream

In this section, you will add an energy stream. Prior to installing the column, an energy stream must be created to represent the trim duty on stage 28 of the main tower.

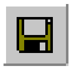


Energy Stream icon

1. Double-click on the **Energy Stream** icon on the **Object Palette**. UniSim Design creates a new energy stream with the default name



Refluxed Absorber icon



Save icon

If you choose to use the pre-built crude column template you still have to customize the column by modifying the various draw and return stages and default specifications. Although using the template eliminates the majority of the work over the next few pages, it is recommended that you work through these pages the first time you build a crude column in UniSim Design. Once you are comfortable working with the side equipment, try using the template. Instructions on using the crude column template are given in an annotation on the next page.

Q-100 and display its property view.

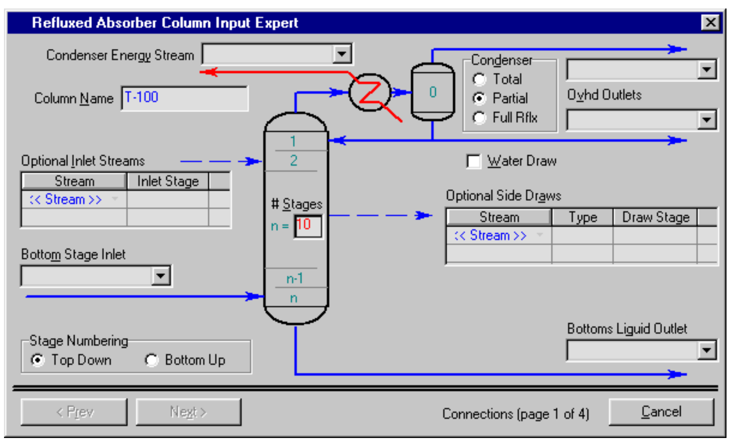
2. In the **Stream Name** field, change the **name** to **Trim Duty**.
3. Close the view.
4. Save your case by doing one of the following:
   - press **CTRL S**.
   - from the **File** menu, select **Save**.
   - click the **Save** icon.

Installing the Column

UniSim Design 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, and adding side equipment. One of these templates is going to be used for this example (a crude column with three side strippers), however, a basic **Refluxed Absorber** column with a total condenser is installed and customized in order to illustrate the installation of the necessary side equipment.

1. Before installing the column, select **Preferences** from the UniSim Design **Tools** menu. Click the **Simulation** tab.
2. On the **Options page**, ensure the **Use Input Experts** checkbox is checked, then close the view.
3. Double-click the **Refluxed Absorber** icon on the **Object Palette.** The first page of the **Input Expert** appears.

Figure 2.77



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

When you install a column using a pre-built template, UniSim Design

To install this column using the pre-built crude column template:

1. Double-click on the **Custom Column** icon on the Object Palette.
2. On the view that appears, click the **Read an Existing Column Template** button. The Available Column Templates view appears, listing the template files ***.col** that are provided in your UniSim Design\template directory. Both 3- and 4-side stripper crude column templates are provided.
3. Select **3sscrude.col** and click the **OK** button. The property view for the new column appears. You can now customize the new column.

supplies certain default information, such as the number of stages. The current active field is **# Stages** (Number of Stages), indicated by the thick border inside this field. There are some other points worth noting:

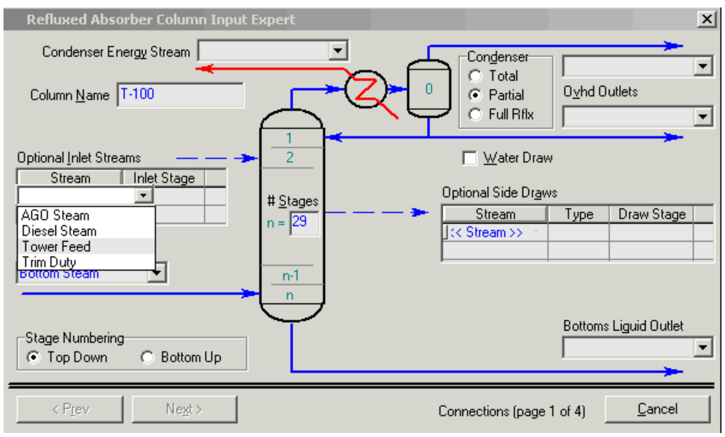
- These are theoretical stages, as the UniSim Design default stage efficiency is one.
- If present, the Condenser and Reboiler are considered separate from the other stages, and are not included in the # Stages field.

Entering Inlet Streams and Number of Trays

For this example, the main column has 29 theoretical stages.

1. Enter **29** in the **# Stages** field.
2. Advance to the **Optional Inlet Streams** table by clicking on the **<<Stream>>** cell, or by pressing **tab**.
3. Click the down arrow to open the drop-down list of available feeds.

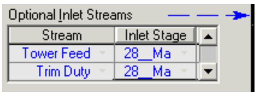
Figure 2.78



4. Select **Tower Feed** as the feed stream to the column. UniSim Design supplies a default feed location in the middle of the Tray Section (TS), in this case stage 15 (indicated by **15_Main TS**). However, the feed stream needs to enter stage 28.
5. In the Optional Inlet Streams group, click in the **Inlet Stage** cell for **TowerFeed**.
6. Type **28** and press **enter**, or select **28_Main TS** from the drop-down list of stages.
7. Click on <**<Stream>**> in the same table, which was automatically advanced down one cell when you attached the Tower Feed stream.

8. From the Stream drop-down list, select the **Trim Duty** stream, which is also fed to stage 28.

Figure 2.79

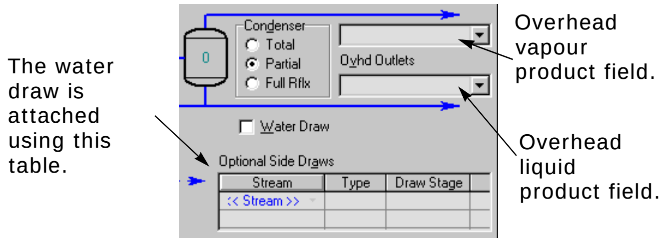


9. Advance to the **Bottom Stage Inlet** field by clicking on it or by pressing **tab**.
10. In the **Bottom Stage Inlet** field, click the down arrow to open the drop-down list of available feeds.
11. From the list, select **Bottom Steam** as the bottom feed for the column.

Entering Outlet Streams

In the **Condenser** group of the Input Expert view, the default condenser type is **Partial**. To the right of this group, there are two **Overhead Outlets**, vapour and liquid. In this case, the overhead vapour stream has no flow, and two liquid phases (hydrocarbon and water) are present in the condenser. The hydrocarbon liquid product is attached in the liquid **Overhead Outlets** field, while the water draw is attached using the **Optional Side Draws** table.

Figure 2.80



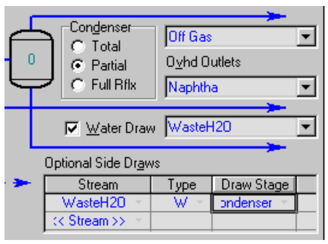
Although the overhead vapour product has zero flow, do not change the condenser to **Total**. At this time, only the **Partial** radio button allows you to specify a three-phase condenser.

1. Click in the top **Ovhd Outlets** field.
2. Enter **Off Gas** as the name of the overhead vapour product stream. UniSim Design creates and attaches a new stream with this name.
3. Press **tab** again to move to the bottom **Ovhd Outlets** field, and enter the new stream name **Naphtha**.

   The next task is to attach the water draw stream to the condenser.

4. In the **Optional Side Draws** table, click in the **<<Stream>>** cell.
5. Enter the name of the draw stream, **WasteH2O**. UniSim Design automatically places a hydrocarbon liquid (indicated by the **L** in the **Type** column) draw on stage 15. You will change this to a condenser water draw.
6. Click on the **Type** cell (the **L**) for the **WasteH2O** stream.
7. Specify a water draw by typing **W** then pressing **enter**, or by selecting W from the drop-down list.
8. Click on the **Draw Stage** cell (**15_Main TS**) for the **WasteH2O** stream.
9. Select **Condenser** from the drop-down list. The condenser is now three-phase.

Figure 2.81

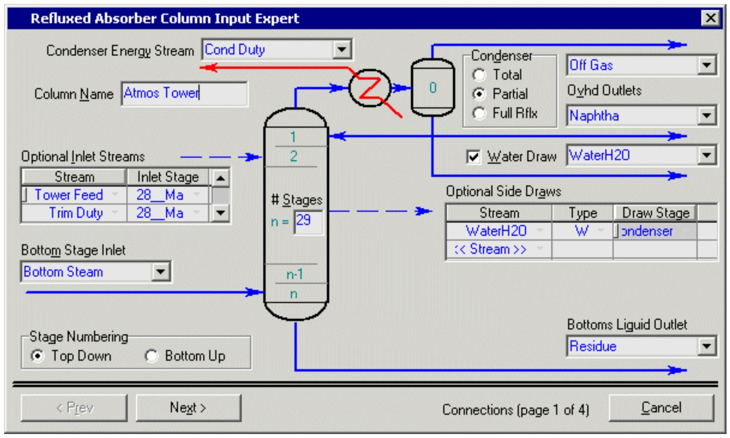


10. In the **Column Name** field, enter **Atmos Tower**.
11. In the **Bottoms Liquid Outlet** field, type **Residue** to create a new stream.
12. In the **Condenser Energy Stream** field, type **Cond Duty** to define a new stream. Press **ENTER**.

All stream attachments made on this page result in the creation of Column sub-flowsheet streams with the same names. For example, when the Main Flowsheet stream **BottomSteam** was attached as a feed, UniSim Design automatically created an identical stream named BottomSteam to be used in the Column sub-flowsheet.

The first page of the Input Expert should appear as shown below.

Figure 2.82



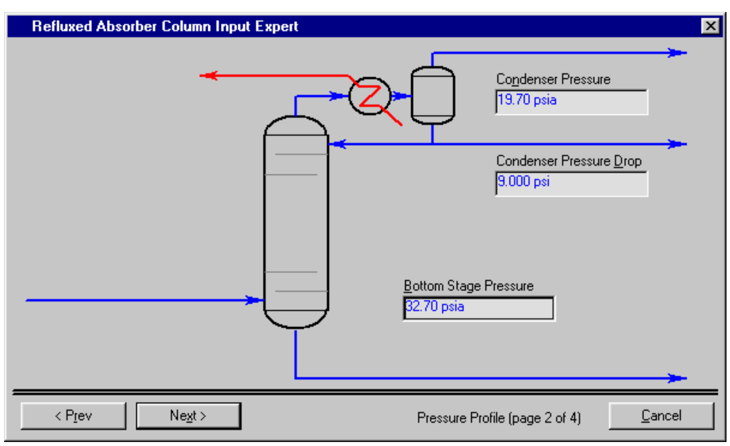
The Next button now becomes available, indicating sufficient information has been supplied to advance to the next page of the **Input Expert**.

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

Entering the Initial Estimate Values

1. On the **Pressure Profile** page, specify the following:
   - Condenser Pressure 19.7 psia
   - Condenser Pressure Drop 9 psi
   - Bottom Stage Pressure 32.7 psia

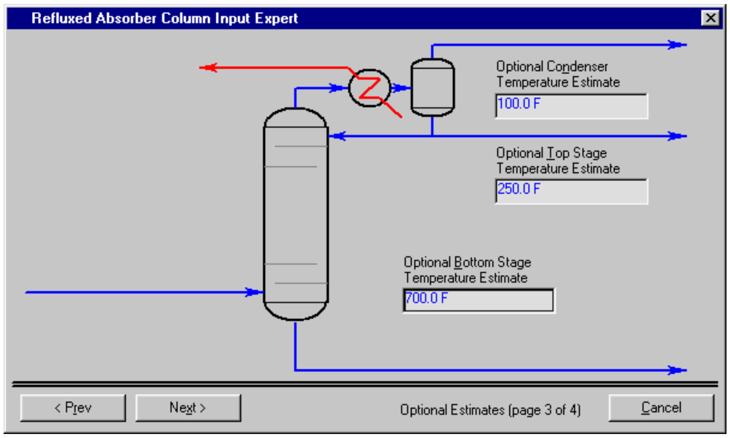
Figure 2.83



2. Click the **Next** button to advance to the **Optional Estimates** page. Although UniSim Design does not usually require estimates to produce a converged column, good estimates result in a faster solution.

3. Specify the following:
   - **Condenser** 100°F
   - **Top Stage** 250°F
   - **Bottom Stage** 700°F

Figure 2.84



4. 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 UniSim Design has created.

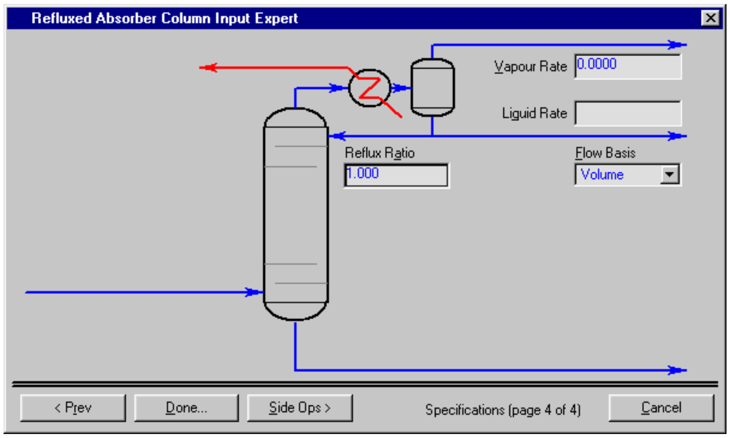
   In general, a refluxed absorber with a partial condenser has two degrees of freedom for which UniSim Design provides two default specifications. For the two specifications given, overhead Vapour Rate is used as an active specification, and **Reflux Ratio** as an estimate only.

5. From the Flow Basis drop-down list, select Volume. All flow specifications are provided in barrels per day.

6. Specify the following:
   - **Vapour Rate 0**

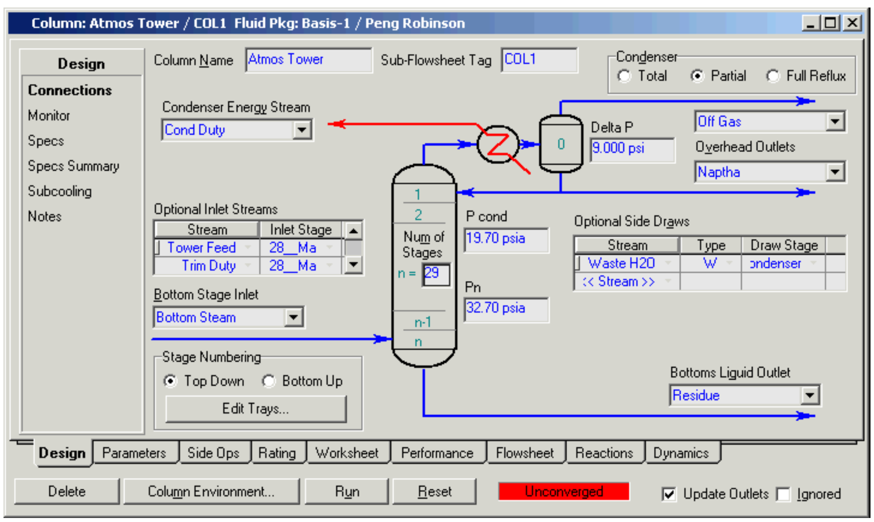
- **Reflux Ratio 1.0**.

Figure 2.85



7. Click the **Done** button. The Column property view appears.

Figure 2.86



Adding Specification Values

1. On the Design tab, select the **Monitor** page.

   The main feature of this page is that it displays the status of your column as it is being calculated, updating information with each iteration. You can also change specification values, and activate or de-activate specifications used by the Column solver, directly from this page.

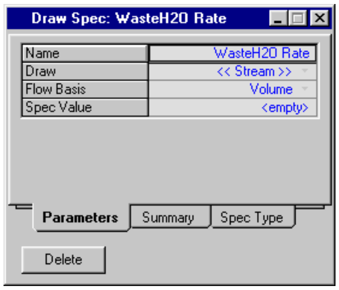
The basic column has three available degrees of freedom. Currently, two Specifications are Active, so the overall Degrees of Freedom is one. The number of available degrees of freedom increases with the addition of side equipment.

The current **Degrees of Freedom** is one, indicating that only two specifications are **active**. As noted earlier, a Refluxed Absorber with a partial condenser has two degrees of freedom and, therefore, requires two **active** specifications. In this case, however, a third degree of freedom was created when the **Trim Duty** stream was attached as a feed, for which the heat flow is unknown. UniSim Design has not made a specification for the third degree of freedom, therefore you need to add a water draw spec called **WasteH2O Rate** to be the third active specification.

2. Select the **Specs** page. Here you will remove two specifications and add one new specification.
3. In the Column Specifications group, select Reflux Rate and then click the **Delete** button.
4. Delete the Btms Prod Rate specification also.
5. Next you will add the WasteH2O Rate specification. Click the **Add** button. The Add Specs view appears.
6. Select Column Draw Rate and click the **Add Spec(s)** button. The Draw Spec property view appears.
7. In the **Name** cell, type WasteH2O Rate. No further information is required as this specification is de-activated and only estimated when you run the column.

The Draw Spec is entered so that the degrees of freedom is kept at zero throughout this tutorial. It is good practice to keep the degrees of freedom at zero as you modify your column so that you can solve the column after every modification.

Figure 2.87



8. Close the view. The new specification appears in the Column Specifications group. The Degrees of Freedom is now zero.
9. Select the **Connections** page. See **Figure 2.86**.

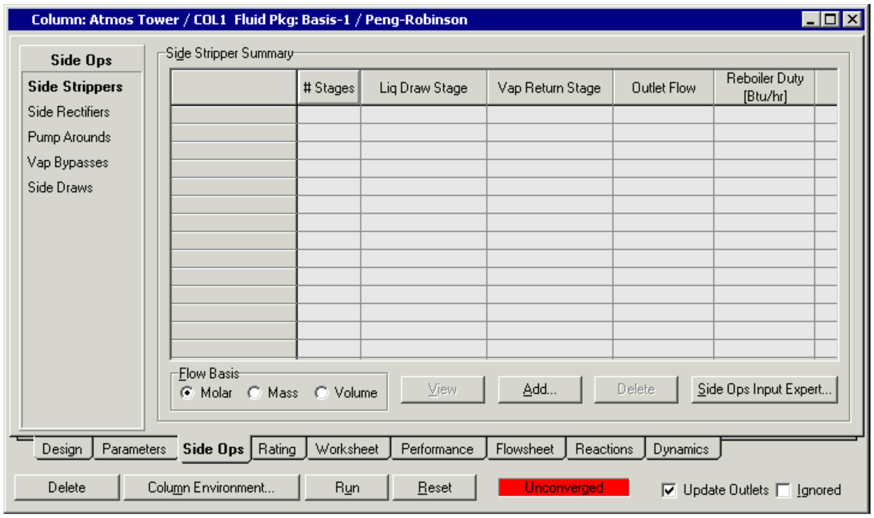
   The Connections page is similar to the first page of the **Input Expert**. Currently, the column is a standard type, so this page shows a column schematic with the names of the attached streams. When the side equipment is added to the column, the page becomes non-standard. There are a large number of possible non-standard columns based on the types and numbers of side operations that are added. Therefore, UniSim Design modifies the **Connections** page into a tabular format, rather than a schematic format, whenever a column becomes non-standard. In the next

section you will add the side equipment and observe how the Connections page is modified.

Installing the Side Strippers

1. Click the **Side Ops** tab of the Column property view.

Figure 2.88

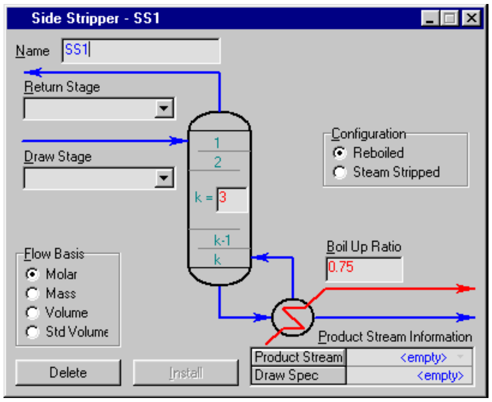


When you install side equipment, it resides in the Column sub-flowsheet. You can build a complex column in the sub-flowsheet while in the Main Flowsheet, the column appears as a single operation. You can then transfer any needed stream information from the sub-flowsheet by simply attaching the stream to the Main Flowsheet.

On this tab, you can Install, View, Edit, or Delete all types of Side Equipment. The table displays summary information for a given type of side operation, depending on the page you are currently on.

2. Ensure that you are on the **Side Strippers** page.
3. Click the **Add** button. The **Side Stripper** view appears.

Figure 2.89

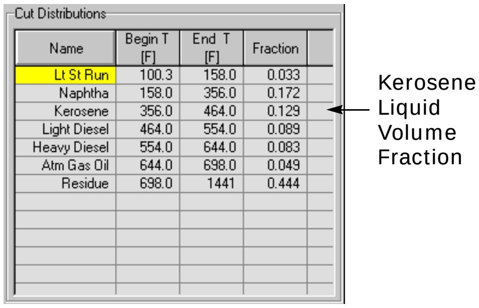


This is a **reboiled** 3-stage stripper with a 0.75 boil up ratio, so leave the **Configuration** radio button at Reboiled, and the **k** = and **Boil Up Ratio** fields at their defaults.

4. In the **Name** field, change the name to **KeroSS**.
5. In the **Return Stage** drop-down list, select stage 8 (**8_Main TS**).
6. In the **Draw Stage** drop-down list, select stage 9 (**9_Main TS**).
7. In the **Flow Basis** group, select the **Std Ideal Vol** radio button.
8. In the **Product Stream fi**eld, enter **Kerosene**.

   The straight run product distribution data calculated during the Oil Characterization appears in the figure below.

Figure 2.90

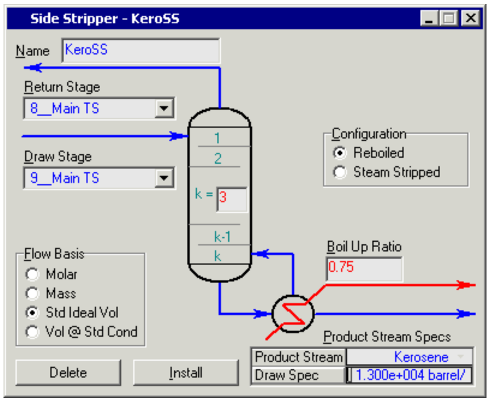

Cut Distributions

Name	Begin T [F]	End T [F]	Fraction
Lt St Run	100.3	158.0	0.033
Naphtha	158.0	356.0	0.172
Kerosene	356.0	464.0	0.129
Light Diesel	464.0	554.0	0.089
Heavy Diesel	554.0	644.0	0.083
Atm Gas Oil	644.0	698.0	0.049
Residue	698.0	1441	0.444

The Kerosene liquid volume fraction is 0.129. For 100,000 bbl/day of crude fed to the tower, Kerosene production can be expected at **100,000 * 0.129 = 12,900** or approximately 13,000 bbl/day.

9. In the **Draw Spec** field, enter **13000**. The completed **Side Stripper** view appears below.

Figure 2.91

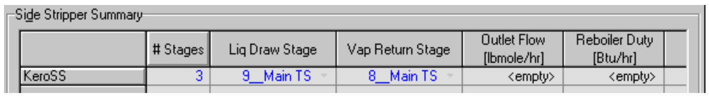


10. Click the **Install** button, and a view summarizing your input appears.

Close icon

11. Click the **Close** icon to return to the Column property view. Summary information for the new side operation appears in the table on the **Side Ops** tab.

Figure 2.92



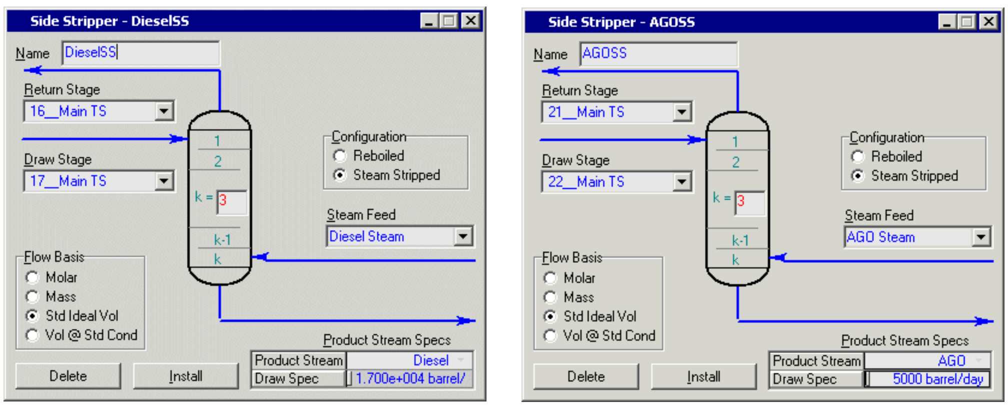
Side Stripper Summary

	# Stages	Liq Draw Stage	Vap Return Stage	Outlet Flow [lbmole/hr]	Reboiler Duty [Btu/hr]
KeroSS	3	9__Main TS	8__Main TS	<empty>	<empty>

12. Use the previous steps to install the two remaining side strippers **DieselSS** and AGOSS. These are both **Steam Stripped**, so choose the appropriate **Configuration** radio button and create the **Steam Feed** and **Product streams** as shown in the following figures. The **@COL1** suffix is added automatically.

    The completed **DieselSS and AGOSS side stripper** views appear in the following figure.

Figure 2.93



Although not a requirement, the names of the Steam Feed streams created for these side strippers are identical to the names of the utility steam streams that were created previously in the Main Flowsheet. The conditions of these Steam Feed streams, which reside in the Column sub-flowsheet, are unknown at this point. The conditions of the Main Flowsheet streams are duplicated into these sub-flowsheet streams when the stream attachments are performed.

The completed **Side Stripper Summary** table appears below.

Figure 2.94

Side Stripper Summary

	# Stages	Liq Draw Stage	Vap Return Stage	Outlet Flow [lbmole/hr]	Reboiler Duty [Btu/hr]
KeroSS	3	9__Main TS	8__Main TS	<empty>	<empty>
DieselSS	3	17__Main TS	16__Main TS	<empty>	<empty>
AGOSS	3	22__Main TS	21__Main TS	<empty>	<empty>

13. Click the **Design** tab and select the **Monitor** page.

    The **Specifications** table on this page has a vertical scroll bar, indicating that new specifications have been created below the default ones. Resize the view to examine the entire table.

14. Click and drag the bottom border of the view down until the scroll bar disappears, making the entire matrix visible.

Figure 2.95

	Specified Value	Current Value	Wt. Error	Active	Estimate	Current
Reflux Ratio	1.000	<empty>	<empty>	☑	☑	☑
Distillate Rate	<empty>	<empty>	<empty>	☑	☑	☑
Vap Prod Rate	0.0000 barrel/day	<empty>	<empty>	☐	☑	☐
WasteH2O	<empty>	<empty>	<empty>	☑	☑	☑
KeroSS Prod Flow	1.300e+004 barrel/day	<empty>	<empty>	☑	☑	☑
KeroSS BoilUp Ratio	0.7500	<empty>	<empty>	☑	☑	☑
DieselSS Prod Flow	1.700e+004 barrel/day	<empty>	<empty>	☑	☑	☑
AGOSS Prod Flow	5000 barrel/day	<empty>	<empty>	☑	☑	☑

The addition of the side strippers has created four more degrees of freedom above the basic column, resulting in a total of seven available degrees of freedom. Currently, however, seven Specifications are Active, so the overall Degrees of Freedom is zero.

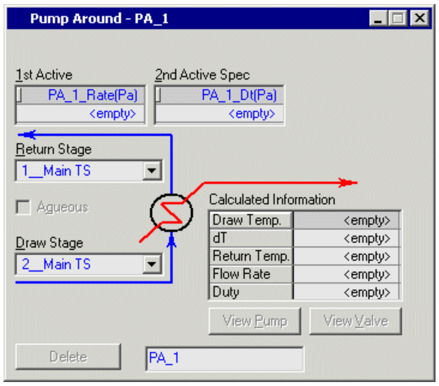
The installation of the side strippers created four additional degrees of freedom, so UniSim Design created a **Prod Flow** (product flow) specification for each side stripper, plus a **BoilUp Ratio** specification for the Kerosene side stripper. The new specifications were automatically made **Active** to exhaust the four degrees of freedom, returning the overall **Degrees of Freedom** to **0**.

Installing the Pump Arounds

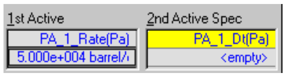
1. Click the **Side Ops** tab and select the **Pump Arounds** page.
2. Click the **Add** button. The initial **Pump Around** view appears.
3. In the **Return Stage** drop-down list, select stage 1 (**1_Main TS**).
4. In the **Draw Stage** drop-down list, select stage 2 (**2_Main TS**).

5. Click the **Install** button, and a more detailed **Pump Around** view appears.

Figure 2.96



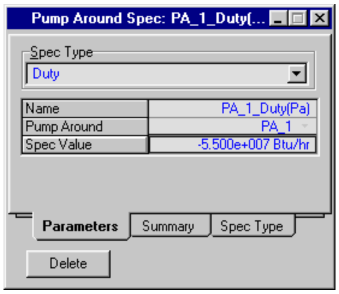
Each cooled pump around circuit has two specifications associated with it. The default **Pump Around Specifications** are circulation rate and temperature drop (**Dt**) between the liquid draw and liquid return. For this example, the **Dt** specification is changed to a Duty specification for the pump around cooler. The pump around rate is 50,000 bbl/day.



6. In the empty cell under the **PA_1_Rate(Pa)** specification, enter **5e4**.
7. Double-click in the blank space under the **PA_1_Dt(Pa)** specification, and the Spec view appears.
8. In the **Spec Type** drop-down list, select **Duty**.
9. in the **Spec Value** cell, enter **-55e6**.

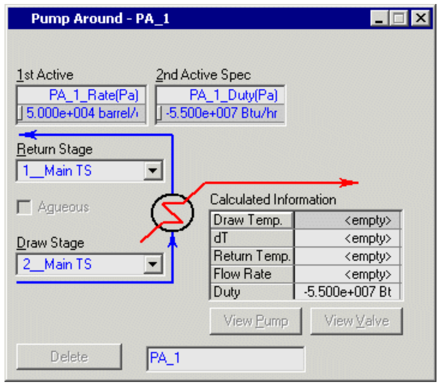
Notice the negative sign convention indicates cooling.

Figure 2.97



10. Click the **Close** icon to return to the **Pump Around** view.

Figure 2.98



The remainder of the information on the above view is calculated by the Column solver.

11. Click the **Close** icon on the main **Pump Around** view to return to the Column property view.

1. Click the **Add** button.
2. Specify the Return Stage and Draw Stage.
3. Click the **Install** button. The second view appears.
4. Specify the 1st Active spec.
5. Double-click the empty cell in the 2nd Active spec.
6. Select Duty from the Spec Type drop-down list.
7. Enter the Spec Value.
8. Close the view.

12. Repeat the previous steps to install the two remaining pump arounds. Enter Rate specifications of **3e4 barrel/day** and **Duty** specifications of **-3.5e7 Btu/hr** for both of these pump arounds.

The completed **Pump Around** views and **Liquid Pump Around Summary** table appear in the following figures.

Figure 2.99

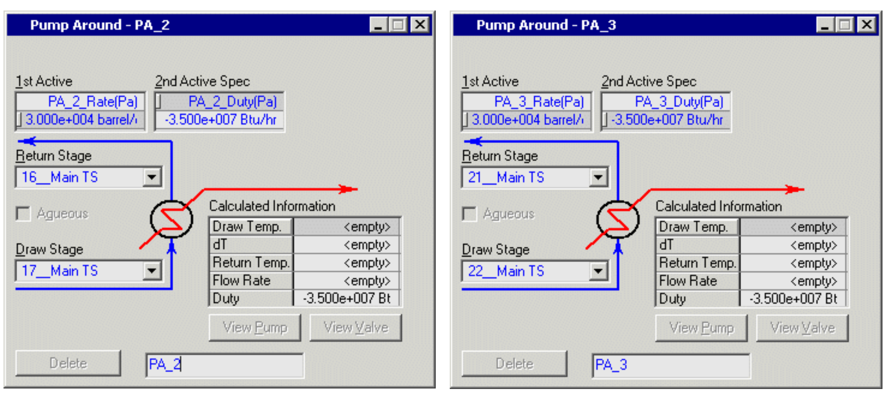


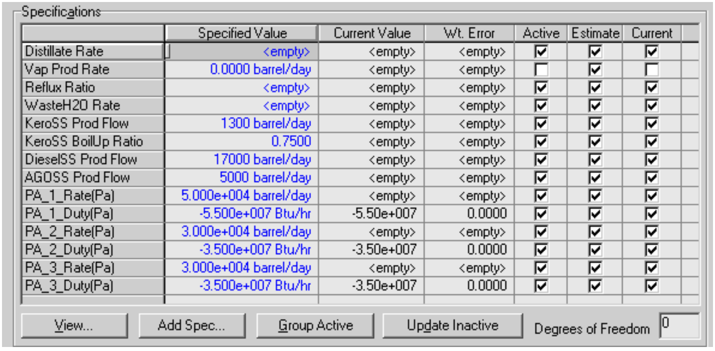
Figure 2.100

Liquid Pump Around Summary

	Draw Stage	Return Stage	Flow [lbmole/hr]	Duty [Btu/hr]	Draw T [F]	Return T [F]	Export
PA_1	2__Main TS	1__Main TS	<empty>	-5.500e+007	<empty>	<empty>	☐
PA_2	17__Main TS	16__Main TS	<empty>	-3.500e+007	<empty>	<empty>	☐
PA_3	22__Main TS	21__Main TS	<empty>	-3.500e+007	<empty>	<empty>	☐

13. Click the **Design tab and select the Monitor** page. Re-size the property view again so the entire **Specifications** table is visible.

Figure 2.101


Specifications

	Specified Value	Current Value	Wt. Error	Active	Estimate	Current
Distillate Rate	<empty>	<empty>	<empty>	☑	☑	☑
Vap Prod Rate	0.0000 barrel/day	<empty>	<empty>	☐	☑	☐
Reflux Ratio	<empty>	<empty>	<empty>	☑	☑	☑
WasteH2O Rate	<empty>	<empty>	<empty>	☑	☑	☑
KeroSS Prod Flow	1300 barrel/day	<empty>	<empty>	☑	☑	☑
KeroSS BoilUp Ratio	0.7500	<empty>	<empty>	☑	☑	☑
DieselSS Prod Flow	17000 barrel/day	<empty>	<empty>	☑	☑	☑
AGOSS Prod Flow	5000 barrel/day	<empty>	<empty>	☑	☑	☑
PA_1_Rate(Pa)	5.000e+004 barrel/day	<empty>	<empty>	☑	☑	☑
PA_1_Duty(Pa)	-5.500e+007 Btu/hr	-5.50e+007	0.0000	☑	☑	☑
PA_2_Rate(Pa)	3.000e+004 barrel/day	<empty>	<empty>	☑	☑	☑
PA_2_Duty(Pa)	-3.500e+007 Btu/hr	-3.50e+007	0.0000	☑	☑	☑
PA_3_Rate(Pa)	3.000e+004 barrel/day	<empty>	<empty>	☑	☑	☑
PA_3_Duty(Pa)	-3.500e+007 Btu/hr	-3.50e+007	0.0000	☑	☑	☑

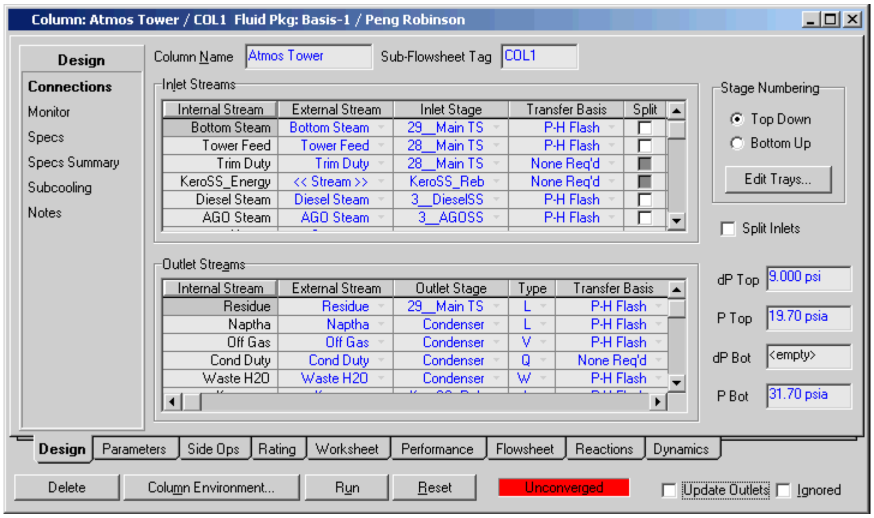
View... | Add Spec... | Group Active | Update Inactive | Degrees of Freedom 0

The addition of the pump arounds has created six more degrees of freedom, resulting in a total of 13 available degrees of freedom. Currently, 13 Specifications are active, so the overall Degrees of Freedom is zero.

The addition of each pump around created two additional degrees of freedom. As with the side strippers, the specifications for the pump arounds have been added to the list and were automatically activated.

14. Select the **Connections** page.

Figure 2.102



The **Connections** page of a standard refluxed absorber property view is essentially identical to the first page of the refluxed absorber **Input Expert**, with a column schematic showing the feed and product streams. Side equipment have been added to the standard refluxed absorber, however, making the column non-standard. The **Connections** page has therefore been modified to show tabular summaries of the **Column Flowsheet Topology** (i.e., all

equipment), **Feed Streams, and Product Streams**.

The column has 40 **Total Theoretical** Stages:

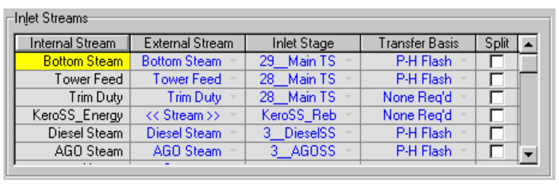
- 29 in the main tray section
- 1 condenser for the main column
- 9 in the side strippers (3 side strippers with 3 stages each)
- 1 reboiler for the Kerosene side stripper

This topology results in 4 **Total Tray Sections**—one for the main column and one for each of the three side strippers.

Completing the Column Connections

When the stream attachments were made on the initial page of the Input Expert, UniSim Design automatically created Column sub-flowsheet streams with the same names. For example, when **Bottom Steam** was attached as a column feed stream, UniSim Design created an identical sub-flowsheet stream named **Bottom Steam**. In the **Inlet Streams** table on the **Connections** page, the Main Flowsheet stream is the **External Stream**, while the sub-flowsheet stream is the **Internal Stream**.

Figure 2.103


Inlet Streams

Internal Stream	External Stream	Inlet Stage	Transfer Basis	Split
Bottom Steam	Bottom Steam	29__Main TS	P-H Flash	
Tower Feed	Tower Feed	28__Main TS	P-H Flash	
Trim Duty	Trim Duty	28__Main TS	None Req'd	
KeroSS_Energy	<< Stream >>	KeroSS_Reb	None Req'd	
Diesel Steam	Diesel Steam	3__DieselSS	P-H Flash	
AGO Steam	AGO Steam	3__AGOSS	P-H Flash	

If you scroll down the list of **Inlet Streams**, notice that the two side stripper steam streams, **DieselSteam** and **AGOSteam**, are **Internal** and External, meaning that these streams are attached to the Main Flowsheet streams that were created earlier.

For the purposes of this tutorial, it is not required to export the pump around duty streams **PA_1_Q, PA_2_Q,** and **PA_3_Q** to the Main Flowsheet, so their **External Stream** cells remain undefined.

Adding Column Specifications

Select the **Monitor** page of the Column property view.

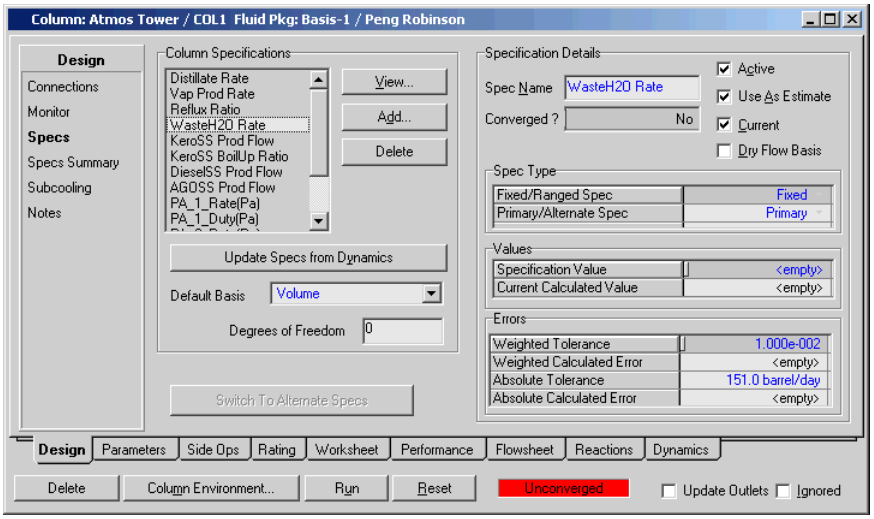
The current **Degrees of Freedom** is zero, indicating the column is ready to be solved. Before you run the column, however, you will have to replace two of the active specifications, **Waste H2O Rate** and **KeroSS BoilUp Ratio**, with the following new ones:

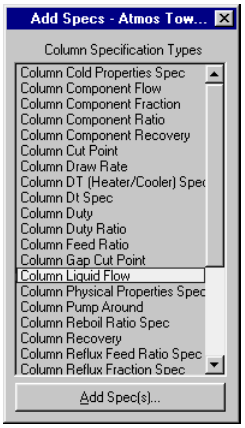
- Overflash specification for the feed stage (Tray Net Liquid Flow specification)
- Kerosene side stripper reboiler duty specification

Adding the Overflash Specification

1. On the **Design** tab, move to the **Specs** page.

Figure 2.104



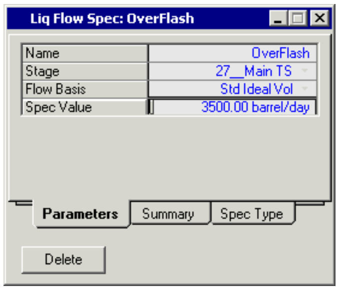


2. In the **Column Specifications** group, click the **Add** button. The **Add Specs** view appears.
3. Select **Column Liquid Flow** as the **Column Specification Type**.
4. Click the **Add Spec(s)** button, and the **Liq Flow Spec** view appears.
5. Change the **name** from its default to **Overflash**.
6. In the **Stage** cell, select **27_Main TS** from the drop-down list of available stages.

   A typical range for the Overflash rate is 3-5% of the total feed to the column. In this case, the total feed rate is 100,000 barrels/day. For the Overflash specification 3.5%, or 3,500 barrels/day is used.

7. In the **Spec Value** cell, enter **3500**.

Figure 2.105

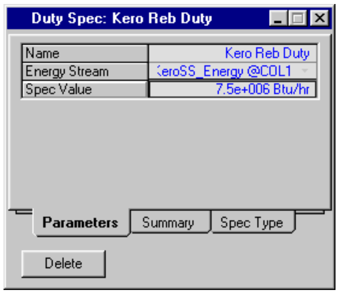


8. Close the view to return to the Column property view. The new specification appears in the list of **Column Specifications** group on the **Specs** page.

Adding the Duty Specification

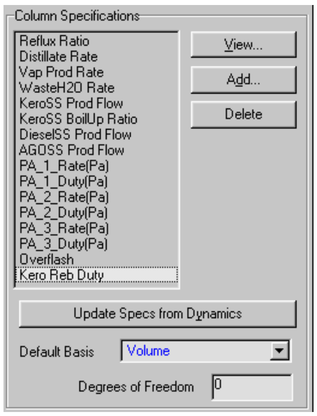
1. Click the **Add** button again to add the second new specification.
2. Select **Column Duty** as the **Column Specification** Type, then click the **Add Spec(s)** button. The **Duty Spec** view appears.
3. In the **Name** cell, change the **name** to **Kero Reb Duty**.
4. In the **Energy Stream** cell, select **KeroSS_Energy @COL1** from the drop-down list.
5. In the **Spec Value** cell, enter **7.5e6** (Btu/hr).

Figure 2.106



6. Close the view to return to the **Specs** page of the Column property view. The completed list of **Column Specifications** is shown in the figure below

Figure 2.107



Running the Column

1. Select the **Monitor** page to view the **Specifications** matrix.

   The **Degrees of Freedom** is again zero, so the column is ready to be calculated, however, a value for the distillate (Naphtha) rate specification must be supplied initially. In addition, there are some specifications which are currently **Active that you want to use** as **Estimates** only, and vice versa.

   Make the following final changes to the specifications:

2. In the **Specified Value** cell for the **Distillate Rate** specification, enter **2e4** (barrel/day).
3. Activate the **Overflash** specification by clicking its **Active** checkbox.
4. Activate the **Kero Reb Duty** specification.
5. Activate the **Vap Prod Rate** specification.
6. Deactivate the **Reflux Ratio** specification.
7. Deactivate the **Waste H2O Rate** specification.
8. Deactivate the **KeroSS BoilUp Ratio** specification.

If the column begins to run on its own before you click the **Run** button, click the **Stop** button and continue activating or deactivating specifications.

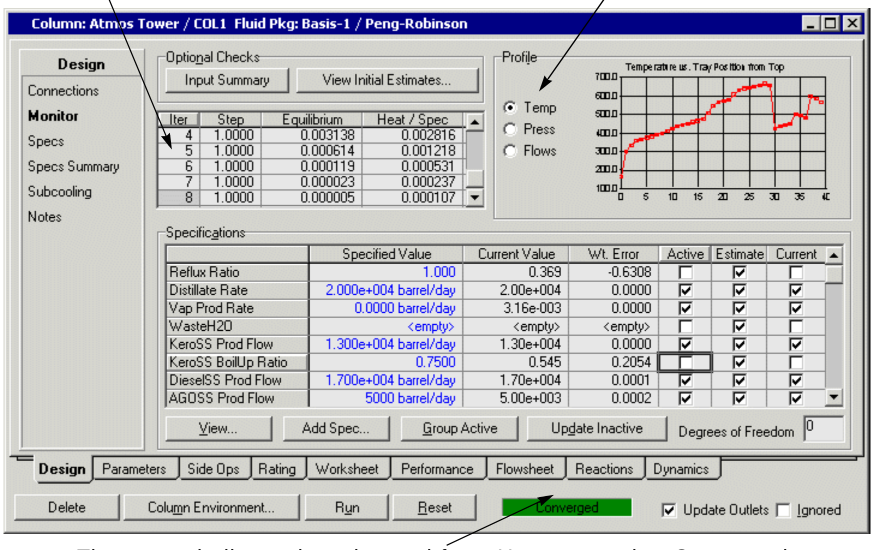
UniSim Design begins calculations and the information displayed on the page is updated with each iteration. The column converges as

shown in the figure below.

Figure 2.108

This matrix displays the Iteration number, Step size, Equilibrium error and Heat/ Spec error.

The column temperature profile is shown here. You can view the pressure or flow profiles by picking the appropriate radio button.



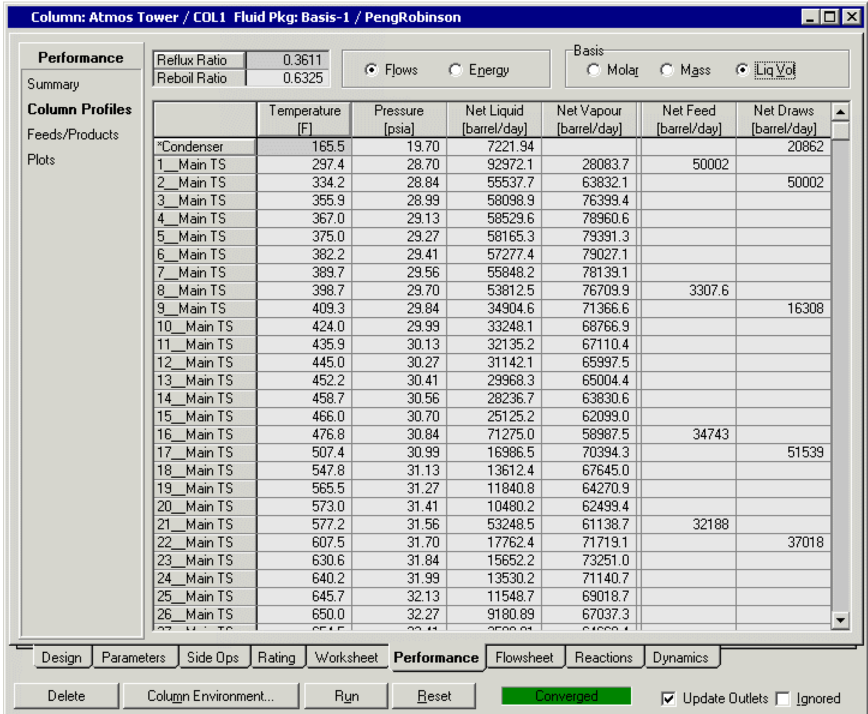
The status indicator has changed from Unconverged to Converged.

The converged temperature profile is currently displayed in the upper right corner of the view. To view the pressure or flow profiles, select the appropriate radio button.

9. Click on the **Performance** tab, then select the **Column Profiles** or **Feed/Products** page to see a more detailed stage summary.

The **Column Profiles** page appears below.

Figure 2.109



	Temperature [F]	Pressure [psia]	Net Liquid [barrel/day]	Net Vapour [barrel/day]	Net Feed [barrel/day]	Net Draws [barrel/day]
*Condenser	165.5	19.70	7221.94			20862
1__Main TS	297.4	28.70	92972.1	28083.7	50002	
2__Main TS	334.2	28.84	55537.7	63832.1		50002
3__Main TS	355.9	28.99	58098.9	76399.4		
4__Main TS	367.0	29.13	58529.6	78960.6		
5__Main TS	375.0	29.27	58165.3	79391.3		
6__Main TS	382.2	29.41	57277.4	79027.1		
7__Main TS	389.7	29.56	55848.2	78139.1		
8__Main TS	398.7	29.70	53812.5	76709.9	3307.6	
9__Main TS	409.3	29.84	34904.6	71366.6		16308
10__Main TS	424.0	29.99	33248.1	68766.9		
11__Main TS	435.9	30.13	32135.2	67110.4		
12__Main TS	445.0	30.27	31142.1	65997.5		
13__Main TS	452.2	30.41	29968.3	65004.4		
14__Main TS	458.7	30.56	28236.7	63830.6		
15__Main TS	466.0	30.70	25125.2	62099.0		
16__Main TS	476.8	30.84	71275.0	58987.5	34743	
17__Main TS	507.4	30.99	16986.5	70394.3		51539
18__Main TS	547.8	31.13	13612.4	67645.0		
19__Main TS	565.5	31.27	11840.8	64270.9		
20__Main TS	573.0	31.41	10480.2	62499.4		
21__Main TS	577.2	31.56	53248.5	61138.7	32188	
22__Main TS	607.5	31.70	17762.4	71719.1		37018
23__Main TS	630.6	31.84	15652.2	73251.0		
24__Main TS	640.2	31.99	13530.2	71140.7		
25__Main TS	645.7	32.13	11548.7	69018.7		
26__Main TS	650.0	32.27	9180.89	67037.3		

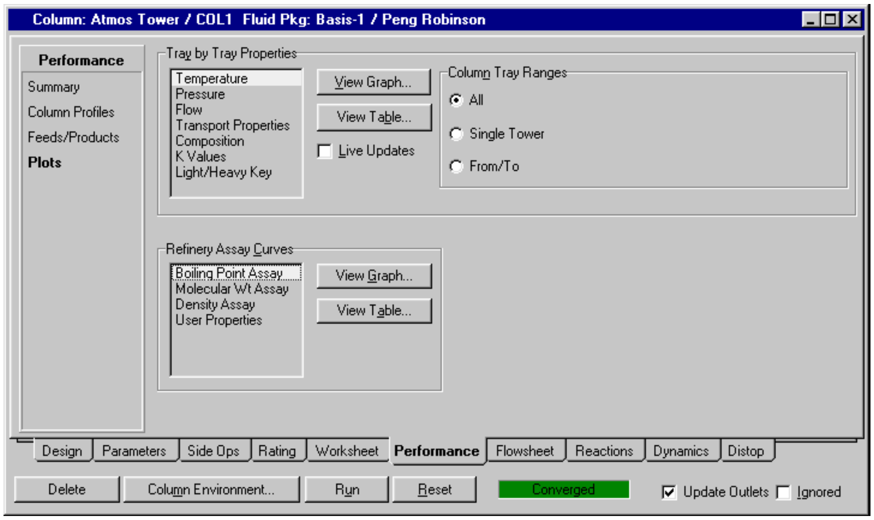
In the Basis group near the top of the view, select the **Liq Vol** radio button to examine the tray vapour and liquid flows on a volumetric basis.

Viewing Boiling Point Profiles for the Product Stream

You can view boiling point curves for all the product streams on a single graph:

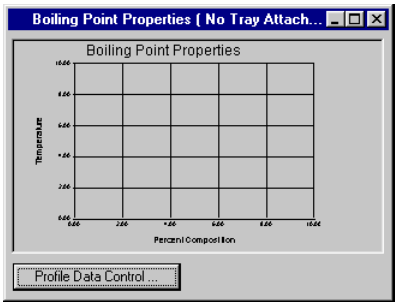
1. On the **Performance** tab, click on the **Plots** page.

Figure 2.110



2. In the **Assay Curves** group, select **Boiling Point Assay**.
3. Click the **View Graph** button, and the **Boiling Point Properties** view appears.

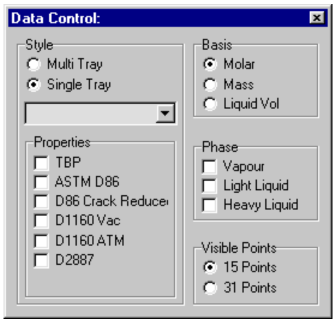
Figure 2.111



No data is plotted on the graph, since there is currently **No Tray Attached**, as shown in the title bar.

4. Click the **Profile Data Control** button, and the **Data Control** view appears as shown below.

Figure 2.112



You can view boiling point properties of a single tray or multiple trays. The boiling point properties of all stages, from which products are drawn, are important for this Tutorial.

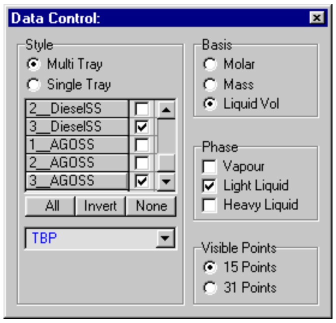
5. Select the **Multi Tray** radio button in the **Style** group. The **Data Control** view is modified, showing a matrix of column stages with a checkbox for each stage.
6. Activate the following stages by clicking on the corresponding checkboxes:
   - Condenser (Naphtha product stage)
   - 29_Main TS (Residue)
   - KeroSS_Reb (Kerosene)
   - 3_DieselSS (Diesel)
   - 3_AGOSS (AGO)

   The TBP profile for the light liquid phase on each stage can be viewed, on a liquid volume basis.
7. Select **TBP** in the drop-down list under the tray matrix in the **Style** group.
8. In the **Basis** group, select the **Liquid Vol** radio button.
9. Activate the **Light Liquid** checkbox in the Phase group to activate it.
10. Leave the **Visible Points** at its default setting of **15 Points**. You can display more data points for the curves by selecting the **31 Points** radio button.

The independent (x-axis) variable is the Assay Volume Percent, while the dependent (y-axis) variable is the TBP in °C.

The completed **Data Control** view is shown below.

Figure 2.113

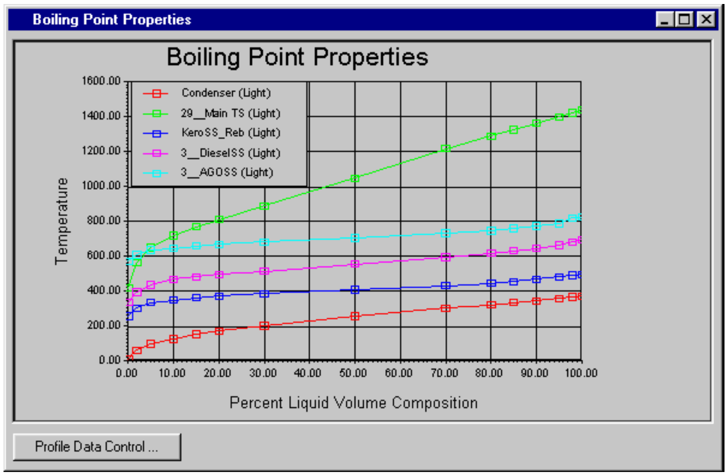


11. Click on the **Close** icon to close the Data Control view. You return to the Boiling Point Properties view, which now displays the TBP curves.
12. Make the **Boiling Point Properties** view more readable by clicking the **Maximize** icon in the upper right corner of the view, or by clicking and dragging its border to a new view size.

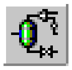
    The Boiling Point Properties view is shown below.

Move the graph legend by double-clicking inside the plot area, then click and drag the legend to its new location.

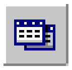
Figure 2.114



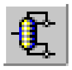
13. When you are finished viewing the profiles, click the **Close** icon.



PFD icon



Workbook icon



Column Runner icon

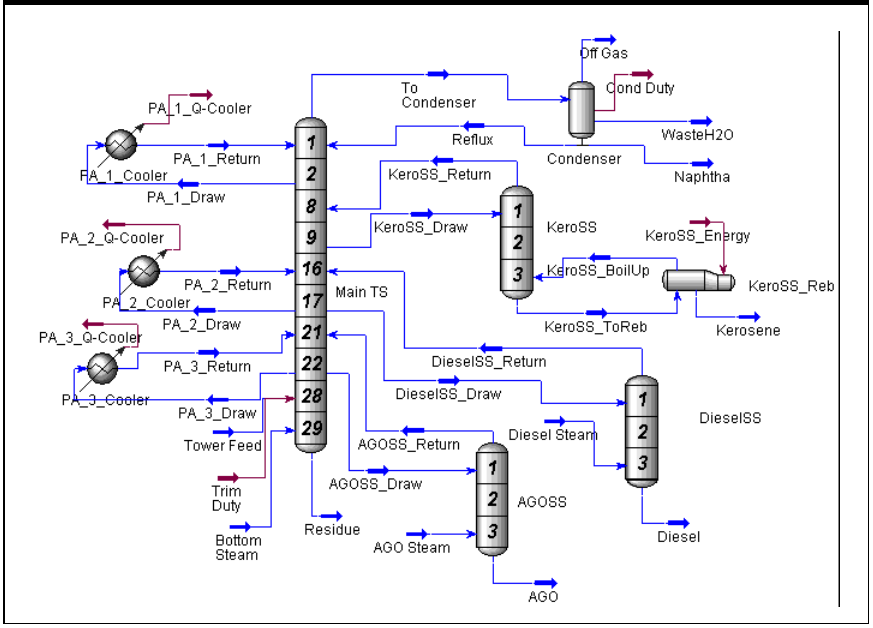
Moving to the Column Sub-Flowsheet

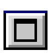
When considering the column, you might want to focus only on the column sub-flowsheet. You can do this by entering the column environment.

1. Click the **Column Environment** button at the bottom of the column property view.
2. While inside the column environment, you might want to:
   - 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.

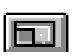
   The Column sub-flowsheet PFD is shown below.

Figure 2.115

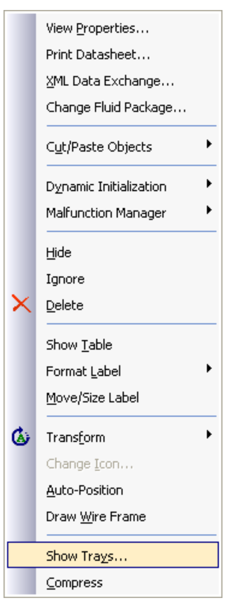




Maximize icon



Zoom All icon



Object Inspect menu

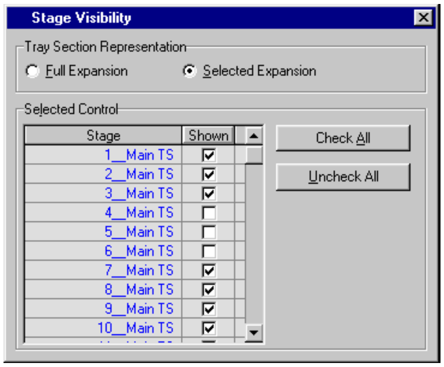
Customizing the Column PFD

You can customize the PFD shown above by re-sizing the column and “hiding” some of the column trays to improve the overall readability of the PFD. To hide some of the trays in the main column:

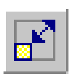
1. Click the **PFD** icon to ensure the column **PFD** is active.
2. Click the **Maximize** icon in the upper right corner of the **PFD** view to make it full-screen.
3. Click the **Zoom All** icon at the bottom left of the **PFD** view to fill the re-sized **PFD** view.
4. Object inspect (right-click) the main column tray section and the object inspection menu appears.
5. Select **Show Trays** from the object inspection menu. The Stage Visibility view appears.

6. Select the **Selected Expansion** radio button.
7. Click the **Check All** button.
8. Hide stages 4, 5, 6, 11, 12, 13, 14, 24, 25, and 26 by deactivating their **Shown** checkboxes.

Figure 2.116

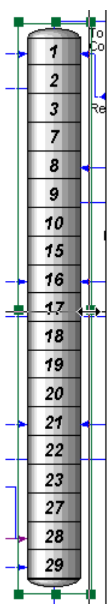


9. Click the **Close** icon on the Stage Visibility view to return to the PFD. The routing of some streams in the **PFD** can be undesirable. You can improve the stream routing by completing the next step.
10. From the **PFD** menu item, select **Auto Position All**, and UniSim Design rearranges the **PFD** in a logical manner.



Size icon

Enlarge Icon



The next task in customizing the **PFD** is to enlarge the icon for the main column:

1. Click on the icon for the main tray section (Main TS).
2. Click the **Size** icon on the PFD button bar, and a frame with eight sizing handles appears around the tray section icon.
3. Place the cursor over the handle at the middle right of the icon, and the cursor changes to a double-ended sizing arrow.
4. With the sizing cursor visible, click and drag to the right. An outline appears, showing what the new icon size is when you complete the next step.
5. When the outline indicates a new icon size of about 1.5 to 2 times the width of the original size, release the button. The tray section icon is now re-sized.
6. Click the **Size** icon again to return to **Move** mode.

The final task is to customize the **PFD** by moving some of the streams and operation labels (names) so they do not overlap. To move a label:

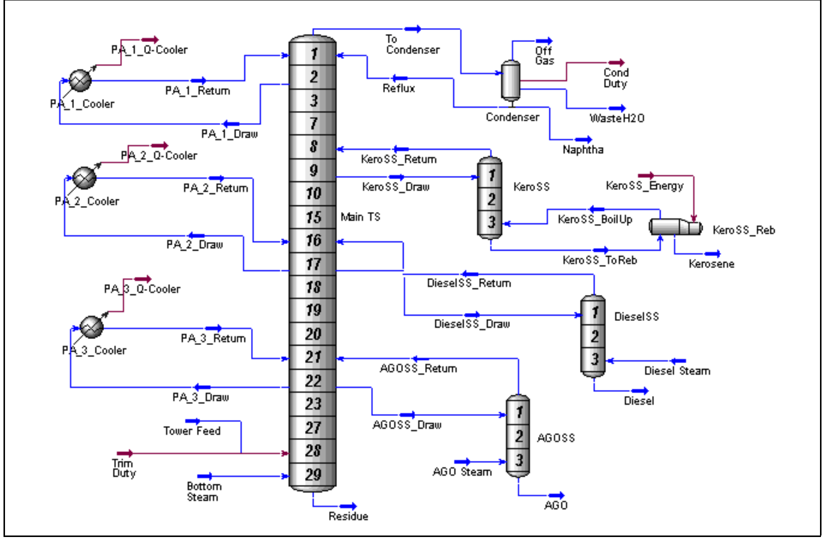
7. Click on the label you want to move.
8. Right-click and select **Move / Size Label**.
9. Move the label to its new position by clicking and dragging it, or by pressing the arrow keys.

   You can also move the icon on its own simply by clicking and dragging it to the new location.
10. When you are finished working with the maximized Column **PFD**, click the **Restore** icon for the **PFD** (not for the UniSim Design Application view) in the upper right corner of the view of the PFD. The **PFD** returns to its previous size.
11. You can manually resize the view, and expand the **PFD** to fill the new size by again clicking the **Zoom All** icon in the lower left corner of the **PFD** view.

   For more information on customizing the PFD, refer to **Section 7.25 - PFD** in the **UniSim Design User Guide**.

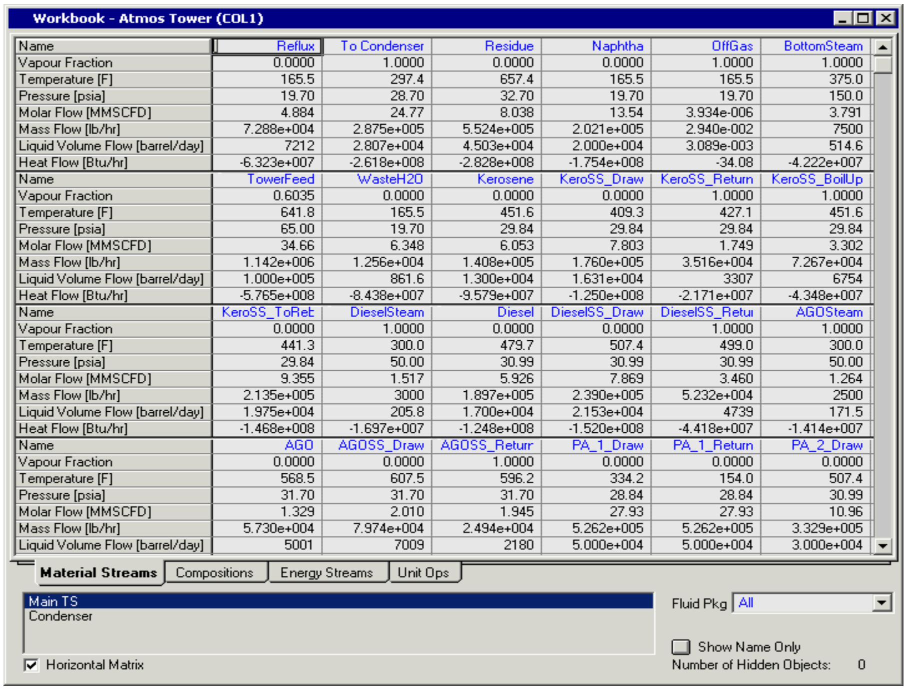
   The customized **PFD** appears below.

Figure 2.117

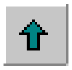


12. To view the workbook for the column, click the **Workbook** icon.

Figure 2.118



Name	Reflux	To Condenser	Residue	Naphtha	OffGas	BottomSteam
Vapour Fraction	0.0000	1.0000	0.0000	0.0000	1.0000	1.0000
Temperature [F]	165.5	297.4	657.4	165.5	165.5	375.0
Pressure [psia]	19.70	28.70	32.70	19.70	19.70	150.0
Molar Flow [MMSCFD]	4.884	24.77	8.038	13.54	3.934e-006	3.791
Mass Flow [lb/hr]	7.288e+004	2.875e+005	5.524e+005	2.021e+005	2.940e-002	7500
Liquid Volume Flow [barrel/day]	7212	2.807e+004	4.503e+004	2.000e+004	3.089e-003	514.6
Heat Flow [Btu/hr]	-6.323e+007	-2.618e+008	-2.828e+008	-1.754e+008	-34.08	-4.222e+007
Name	TowerFeed	WasteH2O	Kerosene	KeroSS_Draw	KeroSS_Return	KeroSS_BoilUp
Vapour Fraction	0.6035	0.0000	0.0000	0.0000	1.0000	1.0000
Temperature [F]	641.8	165.5	451.6	409.3	427.1	451.6
Pressure [psia]	65.00	19.70	29.84	29.84	29.84	29.84
Molar Flow [MMSCFD]	34.66	6.348	6.053	7.803	1.749	3.302
Mass Flow [lb/hr]	1.142e+006	1.256e+004	1.408e+005	1.760e+005	3.516e+004	7.267e+004
Liquid Volume Flow [barrel/day]	1.000e+005	861.6	1.300e+004	1.631e+004	3307	6754
Heat Flow [Btu/hr]	-5.765e+008	-8.438e+007	-9.579e+007	-1.250e+008	-2.171e+007	-4.348e+007
Name	KeroSS_ToRet	DieselSteam	Diesel	DieselSS_Draw	DieselSS_Retu	AGOSteam
Vapour Fraction	0.0000	1.0000	0.0000	0.0000	1.0000	1.0000
Temperature [F]	441.3	300.0	479.7	507.4	499.0	300.0
Pressure [psia]	29.84	50.00	30.99	30.99	30.99	50.00
Molar Flow [MMSCFD]	9.355	1.517	5.926	7.869	3.460	1.264
Mass Flow [lb/hr]	2.135e+005	3000	1.897e+005	2.390e+005	5.232e+004	2500
Liquid Volume Flow [barrel/day]	1.975e+004	205.8	1.700e+004	2.153e+004	4739	171.5
Heat Flow [Btu/hr]	-1.468e+008	-1.697e+007	-1.248e+008	-1.520e+008	-4.418e+007	-1.414e+007
Name	AGO	AGOSS_Draw	AGOSS_Returr	PA_1_Draw	PA_1_Return	PA_2_Draw
Vapour Fraction	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
Temperature [F]	568.5	607.5	596.2	334.2	154.0	507.4
Pressure [psia]	31.70	31.70	31.70	28.84	28.84	30.99
Molar Flow [MMSCFD]	1.329	2.010	1.945	27.93	27.93	10.96
Mass Flow [lb/hr]	5.730e+004	7.974e+004	2.494e+004	5.262e+005	5.262e+005	3.329e+005
Liquid Volume Flow [barrel/day]	5001	7009	2180	5.000e+004	5.000e+004	3.000e+004



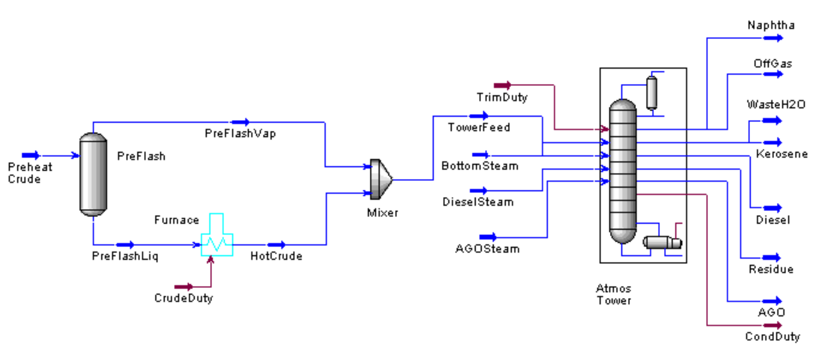
Enter Parent Simulation Environment icon

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

14. Open the **PFD** for the Main Flowsheet, then select **Auto Position All** from the **PFD** menu item. UniSim Design arranges the Main Flowsheet **PFD** in a logical manner according to the layout of the flowsheet.

The **PFD** shown in the **Figure 2.119** has been manually rearranged by moving some of the stream icons, and by enlarging the furnace icon.

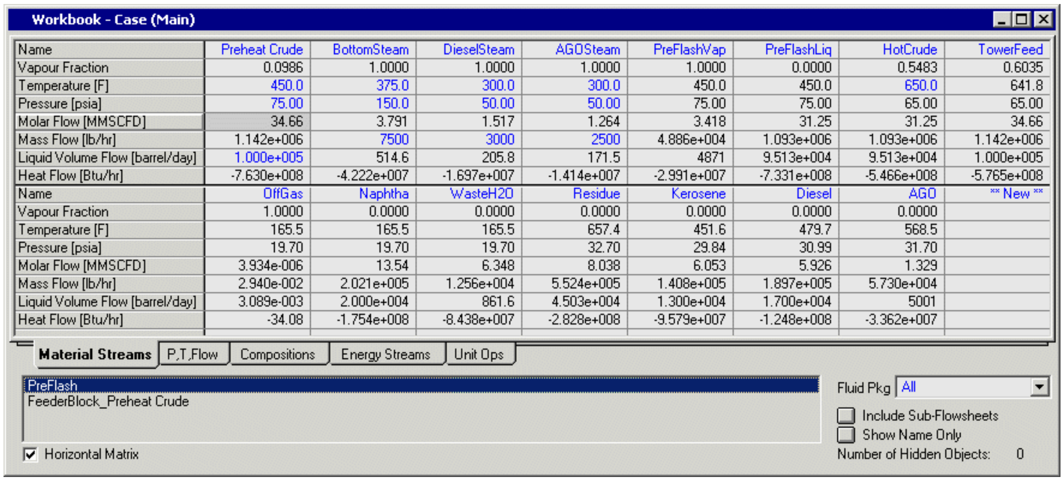
Figure 2.119



2.2.9 Viewing and Analyzing Results

1. Open the **Workbook** to access the calculated results for the Main Flowsheet. The **Material Streams** tab of the **Workbook** appears below.

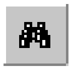
Figure 2.120



Name	Preheat Crude	BottomSteam	DieselSteam	AGOSteam	PreFlashVap	PreFlashLiq	HotCrude	TowerFeed
Vapour Fraction	0.0986	1.0000	1.0000	1.0000	1.0000	0.0000	0.5483	0.6035
Temperature [F]	450.0	375.0	300.0	300.0	450.0	450.0	650.0	641.8
Pressure [psia]	75.00	150.0	50.00	50.00	75.00	75.00	65.00	65.00
Molar Flow [MMSCFD]	34.66	3.791	1.517	1.264	3.418	31.25	31.25	34.66
Mass Flow [lb/hr]	1.142e+006	7500	3000	2500	4.886e+004	1.093e+006	1.093e+006	1.142e+006
Liquid Volume Flow [barrel/day]	1.000e+005	514.6	205.8	171.5	4871	9.513e+004	9.513e+004	1.000e+005
Heat Flow [Btu/hr]	-7.630e+008	-4.222e+007	-1.697e+007	-1.414e+007	-2.991e+007	-7.331e+008	-5.466e+008	-5.765e+008
Name	OffGas	Naphtha	WasteH20	Residue	Kerosene	Diesel	AGO	** New **
Vapour Fraction	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
Temperature [F]	165.5	165.5	165.5	657.4	451.6	479.7	568.5	
Pressure [psia]	19.70	19.70	19.70	32.70	29.84	30.99	31.70	
Molar Flow [MMSCFD]	3.934e-006	13.54	6.348	8.038	6.053	5.926	1.329	
Mass Flow [lb/hr]	2.940e-002	2.021e+005	1.256e+004	5.524e+005	1.408e+005	1.897e+005	5.730e+004	
Liquid Volume Flow [barrel/day]	3.089e-003	2.000e+004	861.6	4.503e+004	1.300e+004	1.700e+004	5001	
Heat Flow [Btu/hr]	-34.08	-1.754e+008	-8.438e+007	-2.828e+008	-9.579e+007	-1.248e+008	-3.362e+007	

Using the Object Navigator

Now that results have been obtained, you can view the calculated properties of a particular stream or operation. The **Object Navigator** allows you to quickly access the property view for any stream or unit operation at any time during the simulation.

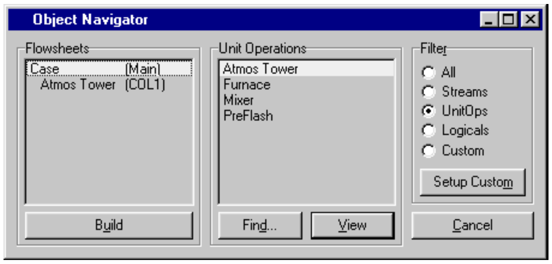


Object Navigator icon

1. Open the Navigator by doing **one** of the following:
   - Press **F3**.
   - From the **Flowsheet** menu, select **Find Object**.
   - Double-click on any blank space on the UniSim Design Desktop.
   - Click the **Object Navigator** icon.

The **Object Navigator** view appears:

Figure 2.121



The **UnitOps** radio button in the **Filter** group is currently selected, so only **Unit Operations** appear in the list of objects. To open a property view, select the operation in the list and click the View button, or double-click on the operation. You can change which objects appear by selecting a different **Filter** radio button. For example, to list all the streams and unit operations, select the **All** radio button.

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** and click the OK button. UniSim Design opens the property view for the object whose name you entered.

2.2.10 Installing a Boiling Point Curves Utility

Previously, the boiling point profiles for the product streams was viewed using the **Plots** page in the column property view. You can also view boiling point curves for a product stream using UniSim Design' BP Curves Utility. To create a Boiling Point Curves utility for the Kerosene product:

1. Open the Navigator using one of the methods described above.
2. Select the **Streams** radio button.
3. Scroll down the list of Streams and select **Kerosene**.
4. Click the **View** button, and the property view for stream **Kerosene** appears.
5. On the **Attachments** tab, move to the **Utilities** page of the stream property view.

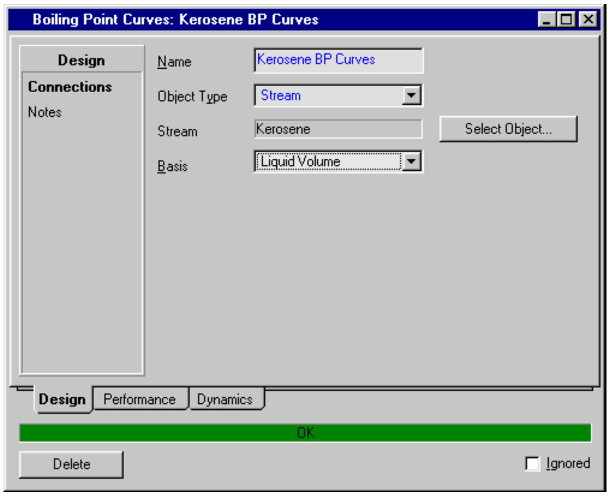
6. Click the **Create** button. The Available Utilities view appears, presenting you with a list of UniSim Design utilities.

Figure 2.122

7. Find BP Curves and do **one** of the following:
   - Select BP Curves, then click the **Add Utility** button.
   - Double-click on BP Curves.
8. UniSim Design creates the utility and opens the Boiling Point Curves view.
9. On the Design tab, go to the **Connections** page. Change the name of the utility from the default Boiling Point Curves-1 to **Kerosene BP Curves**.
10. Change the curve basis to **Liquid Volume** by selecting it from the **Basis** drop-down list.

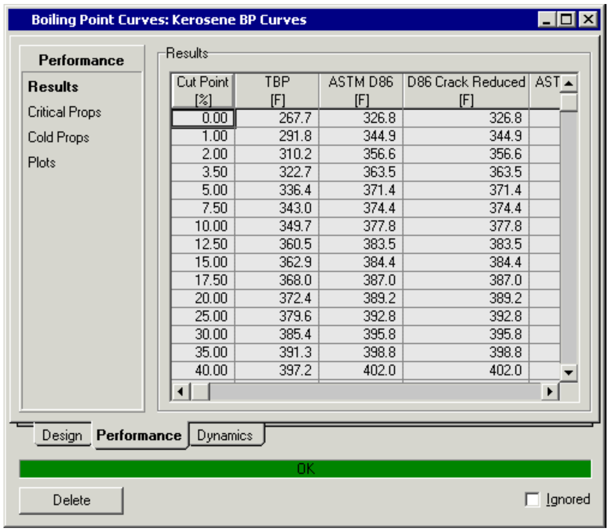
A Utility is a separate entity from the stream it is attached to; if you delete it, the stream is not affected. Likewise, if you delete the stream, the Utility remains but cannot display any information until you attach another stream using the Select Object button.

Figure 2.123



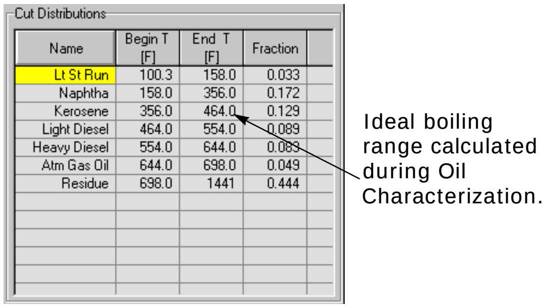
11. You can scroll through the matrix of data to see that the **TBP** ranges from 267°F to 502°F by going to the **Performance** tab and selecting the **Results** page.

Figure 2.124



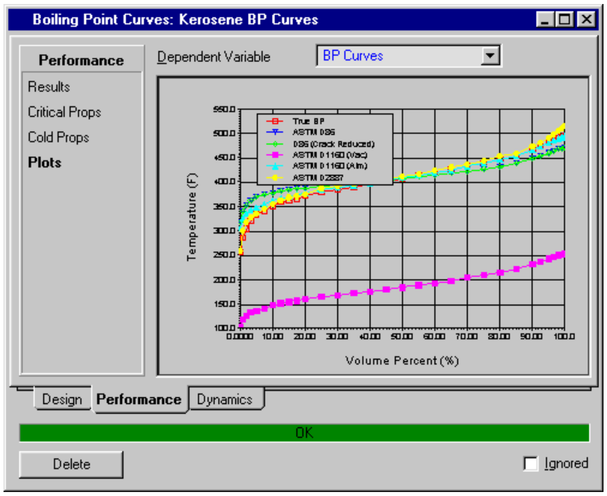
This boiling range predicted by the utility is slightly wider than the ideal range calculated during the Oil characterization procedure for Kerosene, 356°F to 464°F.

Figure 2.125



12. Select the **Plots** page on the **Parameters** tab of the utility property view to view the data in graphical format.

Figure 2.126



To make the envelope more readable, maximize or resize the view.

13. When you move to the **Plots** view, the graph legend can overlap the plotted data. To move the legend, double-click anywhere in the plot area then click and drag the legend to its new location.
14. When you are finished viewing the **Boiling Point Curves**, click the **Close** icon.

Installing a Second Boiling Point Curves Utility

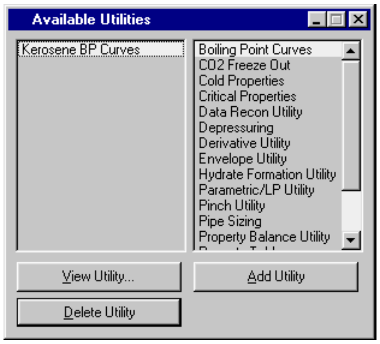
Alternative to using the **Utilities** page of a stream property view, you can also install a utility using the **Available Utilities** view. Another **BP** Curves utility is installed for stream **Residue**. This utility is used for the case study in the next section. To install the utility:

1. Do one of the following:
    - press **CTRL U**.
    - from the **Tools** menu, select **Utilities**.

Notice the name of the utility created previously, Kerosene BP Curves, appears in the Available Utilities view.

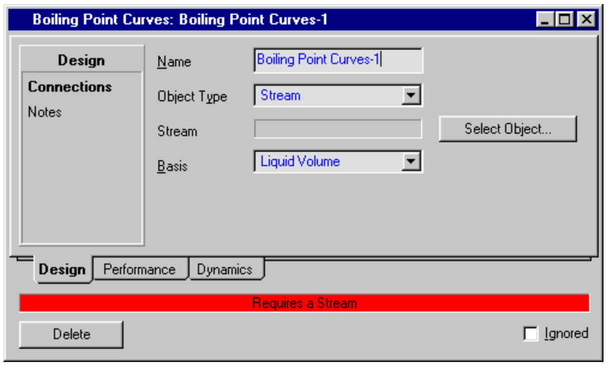
The Available Utilities view appears.

Figure 2.127



2. Select Boiling Point Curves and click the **Add Utility** button. The Boiling Point Curves view appears, opened to the **Design** tab.

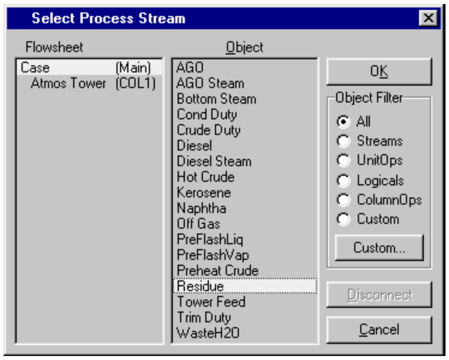
Figure 2.128



3. Change the name from its default Boiling Point Curves-1 to Residue BP Curves.
4. Change the Basis to **Liquid Volume** by selecting it in the drop-down list. The next task is to attach the utility to a material stream.

5. Click the **Select Object** button, and the Select Process Stream view appears.

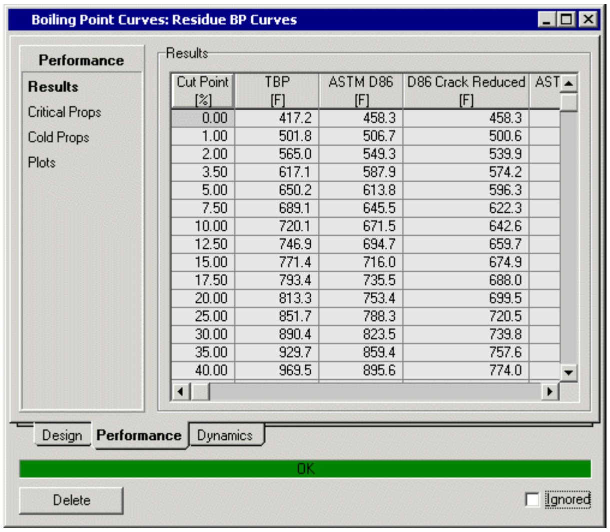
Figure 2.129



6. Select Residue in the Object list, then click the **OK** button. UniSim Design calculates the boiling point curves. The completed **Performance** tab appears below.

Notice that the stream name Residue now appears in the Stream cell.

Figure 2.130



7. Click the **Close** icon on the Residue BP Curves view, and then on the Available Utilities view.

2.2.11 Using the Databook

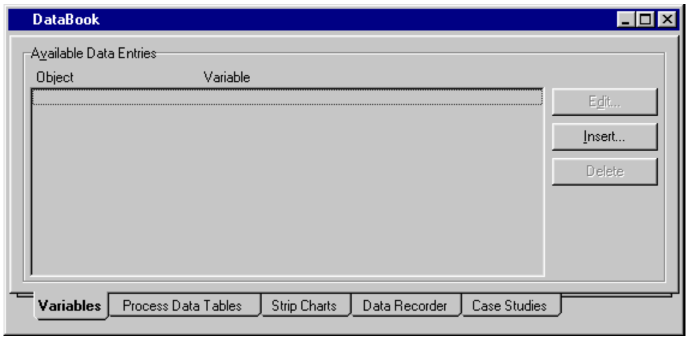
The UniSim Design **Databook** provides you with a convenient way to examine your flowsheet in more detail. You can use the **Databook** to monitor key variables under a variety of process scenarios, and view

the results in a tabular or graphical format.

1. To open the **Databook**, do **one** of the following:
   - press **CTRL D**.
   - from the **Tools** menu, select **Databook**.

   The Databook appears below.

Figure 2.131



Adding Variables to **Databook**

The first step is to add the key variables to the **Databook** using the **Variables** tab. For this example, the Overflash specification is varied and examined to investigate its effect on the following variables:

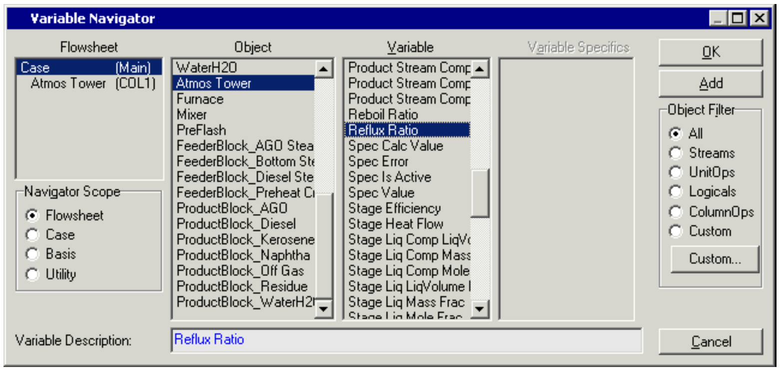
- D1160 Boiling Temperature for 5% volume cut point of stream Residue
- heat flow of energy stream Trim Duty
- column reflux ratio

1. Click the **Insert** button and the Variable Navigator view appears.
2. Select the **UnitOps** radio button in the Object Filter group. The Object list is filtered to show unit operations only.
3. Select Atmos Tower in the Object list, and the Variable list available for the column appears to the right of the Object list.

The Variable Navigator is used extensively in UniSim Design 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.

4. Select Reflux Ratio in the Variable list.

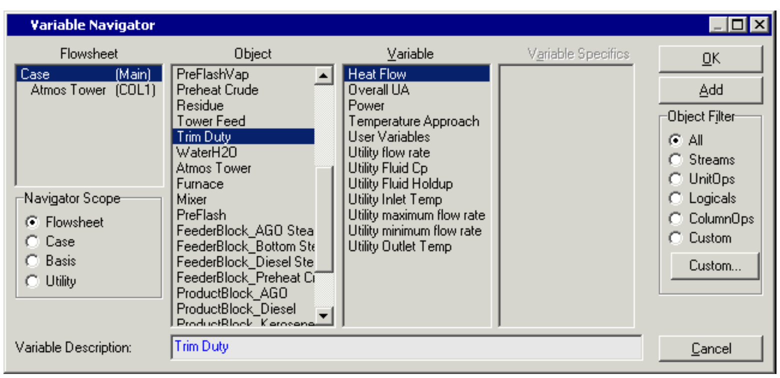
Figure 2.132



5. Click the **Add** button. The variable appears in the Databook and the Variable Navigator view remains open.
6. To add the next variable, select the **Streams** radio button in the **Object Filter** group. The **Object** list is filtered to show streams only.
7. Scroll down and click on **Trim Duty** in the **Object** list, and the **Variable** list available for energy streams appears to the right of the Object list.
8. Select **Heat Flow** in the **Variable** list.

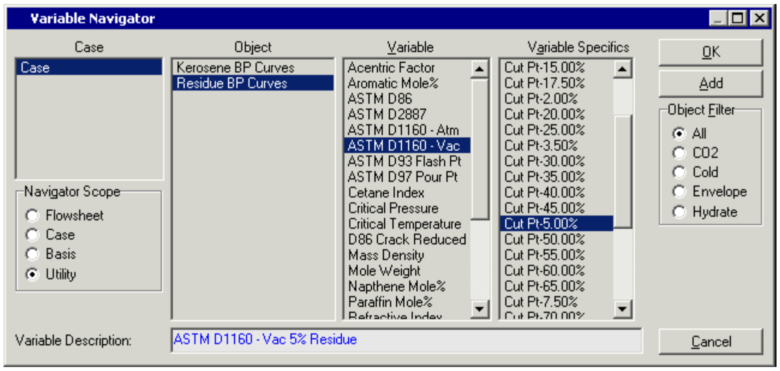
   The variable name is duplicated in the Variable Description field. If you want, you can edit the default description. To edit the default description:
9. Click inside the **Variable Description** field and delete the default name.
10. Type a new description, such as **Trim Duty**, and click the **Add** button. The variable now appears in the Databook.

Figure 2.133



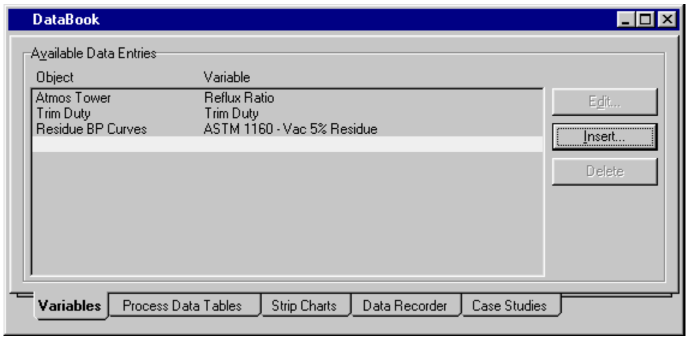
11. To add the third variable, the ASTM D1160 cut point from the **Residue BP Curves** utility, select the **Utility** radio button in the **Navigator Scope** group.
12. Select **Residue BP Curves** in the **Object** list.
13. Select **ASTM D1160 - Vac** in the **Variable** list.
14. Select Cut PT-5.00% in the **Variable Specifics** column. This corresponds to the 5% volume cut point.
15. In the **Variable Description** field, change the variable name to **ASTM 1160 - Vac 5% Residue**, and click the **Close** button.

Figure 2.134



16. The completed **Variables** tab of the **Databook** appears below.

Figure 2.135

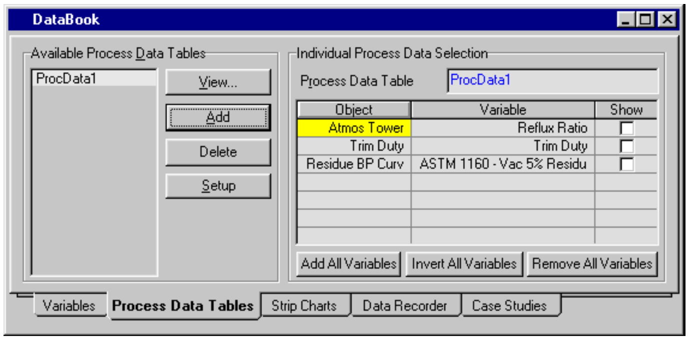


Create a Data Table

Now that the key variables to the **Databook** have been added, the next task is to create a data table to display those variables:

1. Click on the **Process Data Tables** tab.
2. Click the **Add** button in the **Available Process Data Tables** group. UniSim Design creates a new table with the default name **ProcData1**.

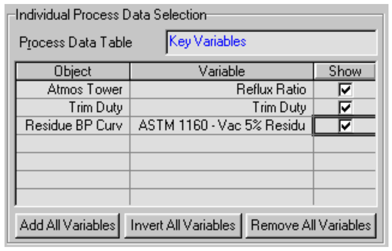
Figure 2.136



3. Change the default name from **ProcData1** to **Key Variables** by editing the **Process Data Table** field.

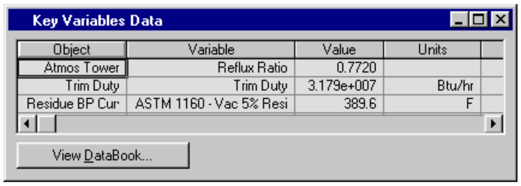
   Notice that the three variables added to the **Databook** appear in the matrix on this tab.
4. Activate each variable by clicking on the corresponding **Show** checkbox.

Figure 2.137



5. Click the **View** button to view the new data table, which is shown below.

Figure 2.138



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

6. For now, click the **Minimize** icon in the upper right corner of the **Key Variables Data** view. UniSim Design reduces the view to an icon and place it at the bottom of the Desktop.

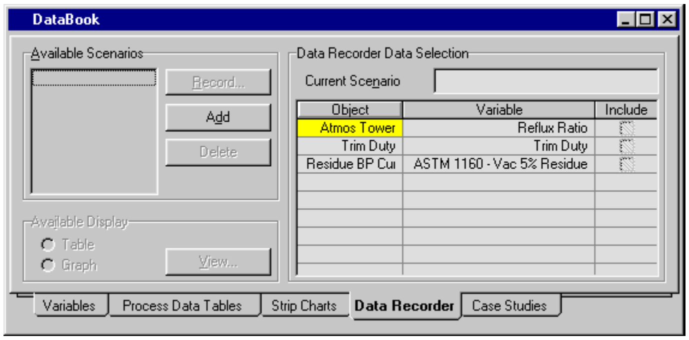
Recording Data

Suppose you now want to make changes to the flowsheet, but you would like to record the current values of the key variables before making any changes. Instead of manually recording the variables, you can use the Data Recorder to automatically record them for you.

To record the current values:

1. Click on the **Data Recorder** tab.

Figure 2.139

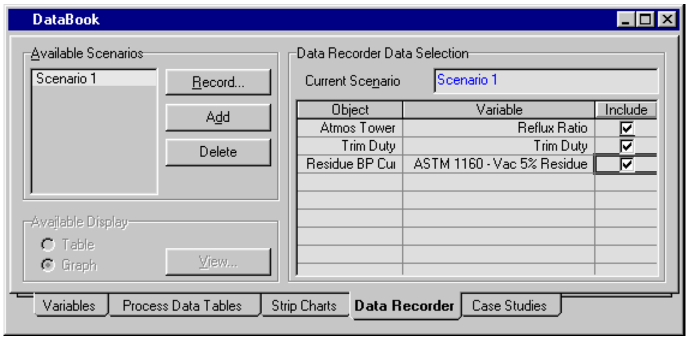


When using the Data Recorder, you first create a **Scenario** containing one or more of the key variables, then record the variables in their current state.

2. Click the **Add** button in the **Available Scenarios** group, and UniSim Design creates a new scenario with the default name **Scenario 1**. It is required to include all three key variables in this scenario.

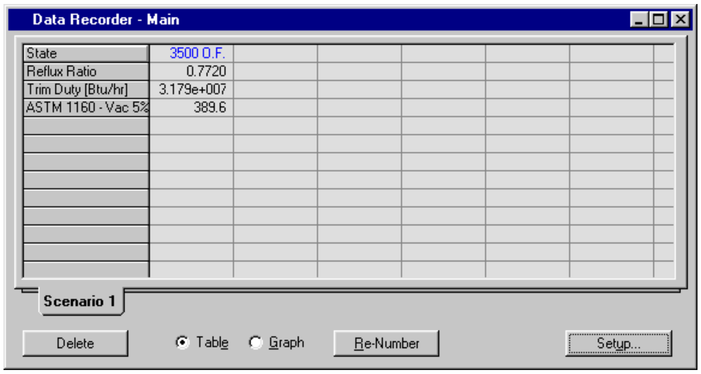
3. Activate each variable by clicking on the corresponding **Include** checkbox.

Figure 2.140



4. 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.
5. Change the **Name for New State** from the default **State 1** to **3500 O.F.** (denoting 3500 bbl/day Overflash). Click the **OK** button and you return to the Databook.
6. In the **Available Display** group, select the **Table** radio button.
7. Click the **View** button and the Data Recorder appears showing the values of the key variables in their current state.

Figure 2.141

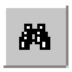


Now you can make the necessary flowsheet changes and these current values remain as a permanent record in the **Data Recorder** unless you choose to erase them.

8. Click the **Minimize** icon to reduce the **Data Recorder** to an icon.

Changing the Overflash Specification

The value of the Overflash specification is going to be changed in the column and the changes is viewed in the process data table:



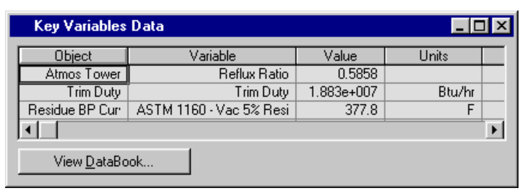
Object Navigator icon

1. Click the **Object Navigator** icon on the toolbar.
2. Select the **UnitOps** radio button in the **Filter** group.
3. Select **Atmos Tower** and click the **View** button. The **Atmos Tower** property view appears.
4. Go to the **Design** tab and select the **Monitor** page.
5. Scroll down to the bottom of the **Specifications** table so the **Overflash** specification is visible.

   A typical range for the Overflash rate is 3-5% of the tower feed. A slightly wider range is examined: 1.5-7.5%, which translates to 1500-7500 bbl/d.

6. Change the **Specified Value** for the **Overflash** specification from its current value of **3500** barrel/day to **1500** barrel/day. UniSim Design automatically recalculates the flowsheet.
7. Double-click on the **Key Variables Data** icon to restore the view to its full size. The updated key variables are shown below.

Figure 2.142



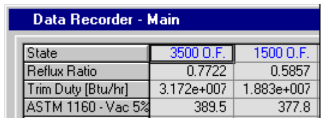
As a result of the change:

- the Trim Duty has decreased
- the Residue D1160 Vacuum Temperature 5% cut point has decreased
- the column reflux ratio has decreased

8. Press **CTRL D** to make the **Databook** active again. You can now record the key variables in their new state.
9. Move to the **Data Recorder** tab in the Databook.
10. Click the **Record** button, and UniSim Design provides you with the default name State 2 for the new state.
11. Change the name to 1500 O.F. and click the **OK** button to accept the new name.

12. Click the **View** button and the **Data Recorder** appears, displaying the new values of the variables.

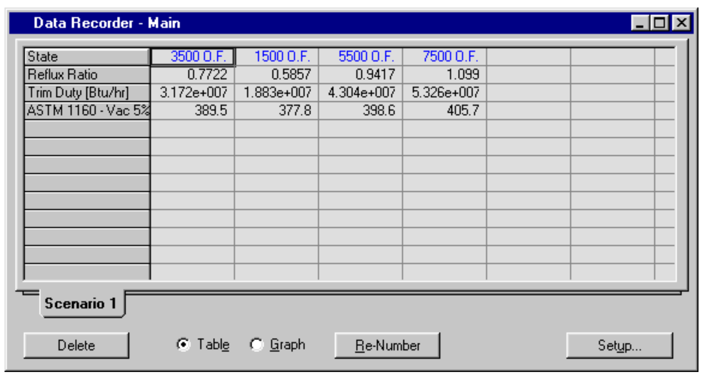
Figure 2.143


Data Recorder - Main

State	3500 O.F.	1500 O.F.
Reflux Ratio	0.7722	0.5857
Trim Duty [Btu/hr]	3.172e+007	1.883e+007
ASTM 1160 - Vac 5%	389.5	377.8

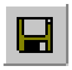
13. Record the process variables for **Overflash** rates of **5500** and **7500** barrels/day. Enter names for these variable states of **5500 O.F.** and **7500 O.F.**, respectively. The final **Data Recorder** appears below.

Figure 2.144


Data Recorder - Main

State	3500 O.F.	1500 O.F.	5500 O.F.	7500 O.F.
Reflux Ratio	0.7722	0.5857	0.9417	1.099
Trim Duty [Btu/hr]	3.172e+007	1.883e+007	4.304e+007	5.326e+007
ASTM 1160 - Vac 5%	389.5	377.8	398.6	405.7

14. Save your case by doing one of the following:
    - press **CTRL S**.
    - from the **File** menu, select **Save**.
    - click the **Save** icon.


Save icon

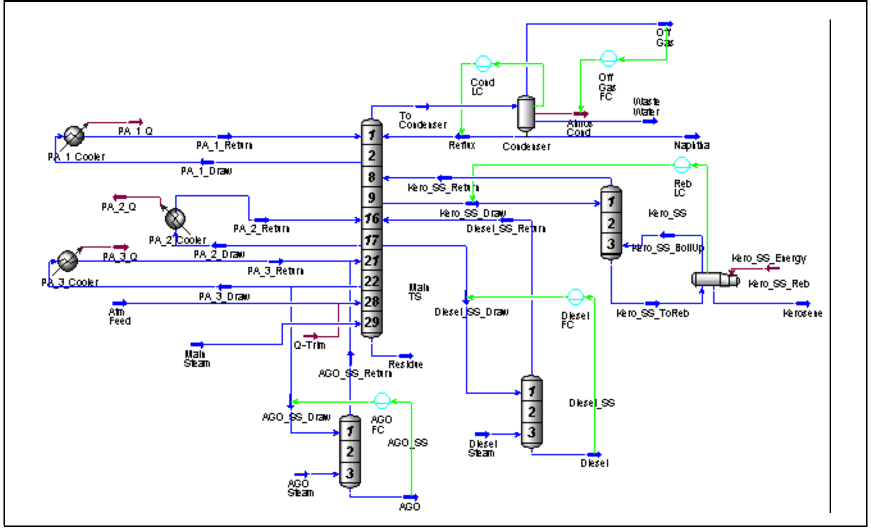
2.3 Dynamic Simulation

This complete dynamic case has been pre-built and is located in the file **DynTUT2.usc** in your UniSim Design\Samples directory.

In this tutorial, the dynamic capabilities of UniSim Design are incorporated into a basic steady state oil refining model. A simple fractionation facility produces naphtha, kerosene, diesel, atmospheric gas oil, and atmospheric residue products from a heavy crude feed. In the steady state refining tutorial, preheated crude was fed into a pre-flash drum which separated the liquid crude from the vapour. The liquid crude was heated in a furnace and recombined with the vapour. The combined stream was then fed to the atmospheric crude column for fractionation. The dynamic refining tutorial only considers the crude column. That is, the crude preheat train is deleted from the flowsheet

and only the crude column in the steady state refining tutorial is converted to dynamics.

Figure 2.145



The main purpose of this tutorial is to provide you with adequate knowledge in converting an existing steady state column to a dynamics column. The tutorial provides a single way of preparing a steady state case for dynamics mode, however, you can also choose to use the Dynamic Assistant to set pressure specifications, size the equipment in the plant, and/or add additional equipment to the simulation flowsheet.

This tutorial comprehensively guides you through the steps required to add dynamic functionality to a steady state oil refinery simulation. To help navigate these detailed procedures, the following milestones have been established for this tutorial.

In this tutorial, you follow this basic procedure in building the dynamic model.

1. Obtain a simplified steady state model to be converted to dynamics.
2. Implement a tray sizing utility for sizing the column and the side stripper tray sections.
3. Install and define the appropriate controllers.
4. Add the appropriate pressure-flow specifications.
5. Set up the Databook. Make changes to key variables in the process and observe the dynamic behaviour of the model.

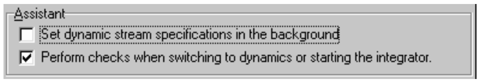
2.3.1 Simplifying the Steady State Flowsheet

In this section, you will delete the preflash train in the steady state simulation case R-1.usc:

1. Open the pre-built case file **R-1.usc**. The crude column simulation file R-1.usc is located in your UniSim Design\Samples directory.
2. Press **F4** to make the Object Palette visible.

   For the purpose of this example, the Session Preferences are set so that the Dynamic Assistant will not manipulate the dynamic specifications.
3. From the **Tools** menu, select **Preferences**. The Session Preference view appears.
4. On the **Simulation** tab, select the **Dynamics** page.
5. Deactivate the **Set dynamic stream specifications in the background** checkbox.

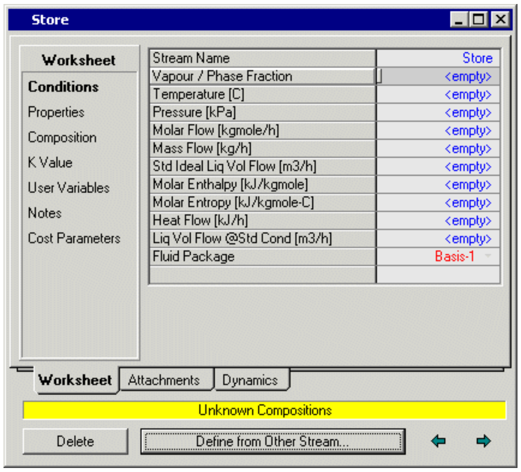
Figure 2.146



In this tutorial, you are working with SI units. The units are changed by entering the Preferences property view in the Tools menu bar. In the Units tab, specify SI in the Current Unit Set group.

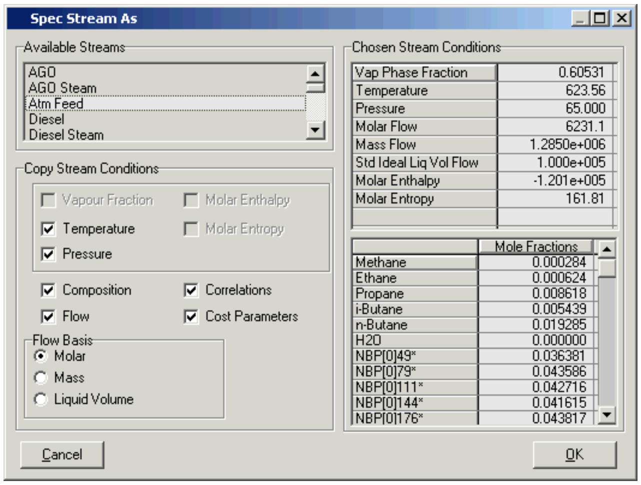
6. Click the **Variables** tab, then select the **Units** page.
7. In the Available Unit Sets group, select SI.
8. Click the **Close** icon to close the Session Preferences view. Close all other views except for the PFD view.
9. Add a material stream to the PFD by doing one of the following:
   - From the **Flowsheet** menu, select **Add Stream**.
   - Double-click the **Material Stream** icon on the Object Palette.
10. In the **Stream Name** cell, type **Store**. This stream will be used to store information from the Atm Feed stream.

Figure 2.147



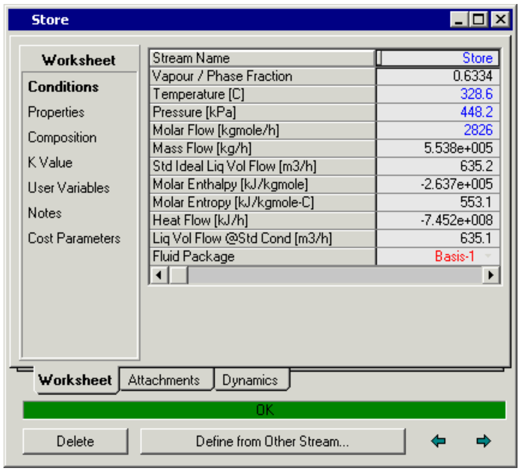
11. In the Store stream property view, click the **Define from Other Stream** button. The Spec Stream As view appears.
12. Select **Atm Feed** in the Source stream group.

Figure 2.148



13. Click on the **OK** button to copy the Atm Feed stream information to the Store stream.

Figure 2.149



14. Close the Store stream view.

When you delete a stream, unit or logical operation from the flowsheet, UniSim Design asks you to confirm the deletion. If you want to delete the object, click the **Yes** button. If not, click the **No** button.

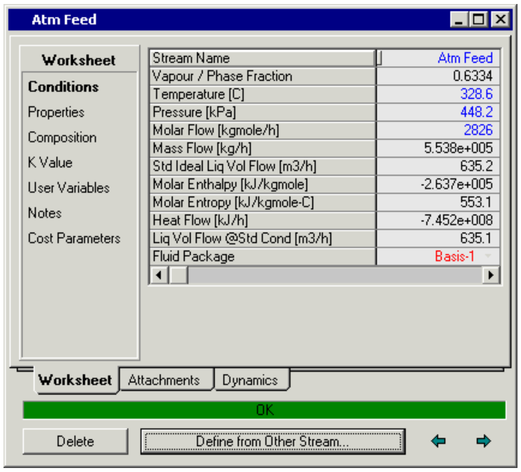
15. Delete all material streams and unit operations upstream of the Atm Feed stream. The following eight items should be deleted:

Items to be deleted		
Material Streams	**Energy Streams**	**Unit Operations**
Hot Crude	Crude Duty	PreFlash Separator
PreFlsh Liq		Crude Heater
PreFlsh Vap		Mixer
Raw Crude		

After you delete the above items, stream Atm Feed is not fully specified.

16. Double-click the **Atm Feed** stream icon to open its property view.
17. Click the **Define from Other Stream** button. The Spec Stream As property view appears.
18. Select **Store** in the Source Stream group and click **OK**.

Figure 2.150



19. Close the Atm Feed stream view, then delete the stream **Store**.

This steady state case now contains the crude column without the preflash train. Since the identical stream information was copied to stream Atm Feed, the crude column operates the same as before the deletion of the preflash train.

20. Save the case as **DynTUT2-1.usc**.

Make sure that the **Standard Windows file picker** radio button is selected on the **File** page in the Session Preferences view.

For more information on Session Preferences please refer to **Section 12.5 - Files Tab** in the **UniSim Design User Guide**.

2.3.2 Adding Equipment & Sizing Columns

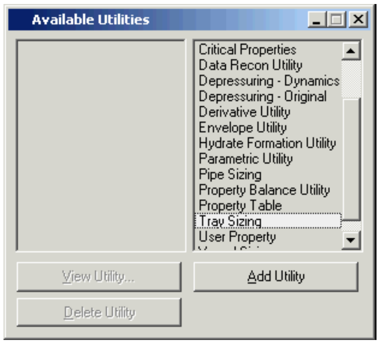
In preparation for dynamic operation, the column and side stripper tray sections and surrounding equipment must be sized. In the steady state scenario, column pressure drop is user specified. In dynamics, it is calculated using dynamic hydraulic calculations. Complications arise in the transition from steady state to dynamics if the steady state pressure profile across the column is very different from that calculated by the Dynamic Pressure-Flow solver.

The Cooler operations in the pump arounds are not specified with the Pressure Flow or Delta P option, however, each cooler must be specified with a volume in order to run properly in dynamic mode.

Column Tray Sizing

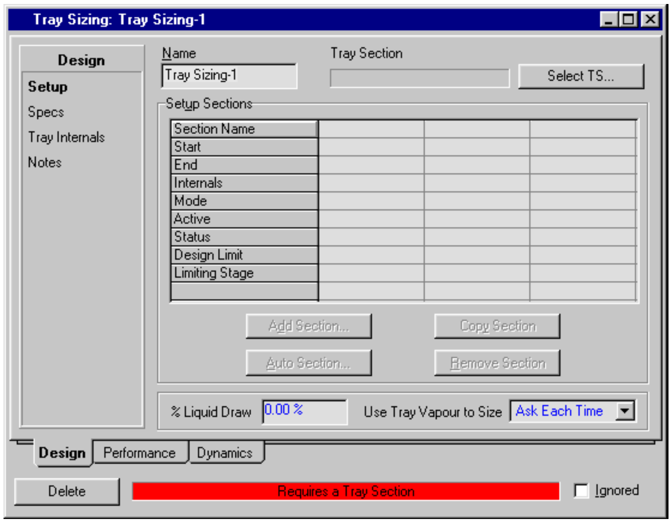
1. Open the Utilities property view by pressing **CTRL U**.
   The Available Utilities view appears.
2. Scroll down the list of available utilities until the Tray Sizing utility is visible.

Figure 2.151



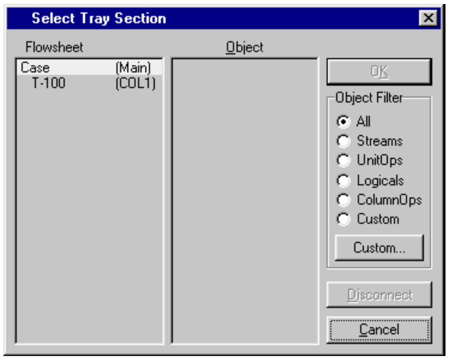
3. Select Tray Sizing, then click the **Add Utility** button. The Tray Sizing view appears.

Figure 2.152



4. In the **Name** field, change the name to **Main TS**.
5. Click the **Select TS** button. The Select Tray Section view appears.

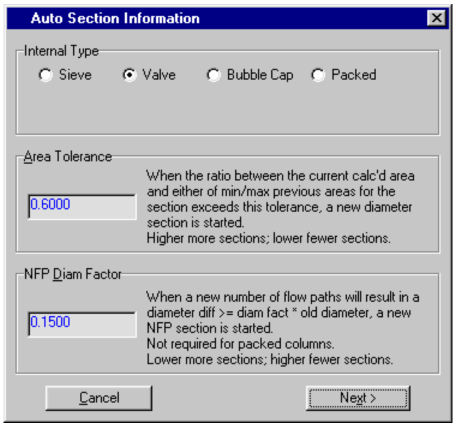
Figure 2.153



6. In the Flowsheet list, select **T-100**, then select **Main TS** in the Object list. Click the **OK** button.
7. In the Use Tray Vapour to Size drop-down list, select **Always Yes**.

8. Click the **Auto Section** button. The Auto Section Information view appears. The default tray internal types appear with the **Valve** type selected.

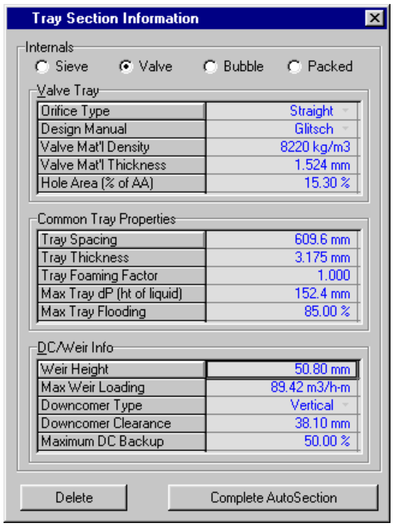
Figure 2.154



The Valve tray type is selected as the default option. This option is entered into the Main TS property view.

9. Keep the default values and click **Next**. The next view displays the specific dimensions of the valve-type trays.
10. Keep the default values and click the **Complete AutoSection** button.

Figure 2.155

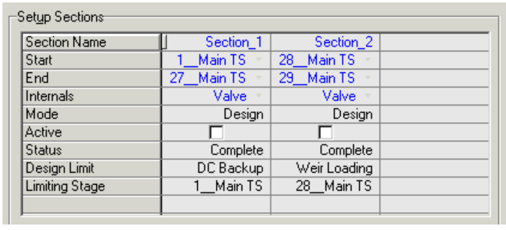


UniSim Design calculates the Main TS tray sizing parameters based on the steady state flow conditions of the column and the desired tray types.

Two tray section sizes, Section_1 and Section_2, appear in the

Setup page of the Design tab. Section_1 includes trays 1 to 27; Section_2 includes trays 28 and 29. Since there are different volumetric flow conditions at each of these sections, two different tray section types are necessary.

Figure 2.156



Setup Sections

Section Name	Section_1	Section_2
Start	1__Main TS	28__Main TS
End	27__Main TS	29__Main TS
Internals	Valve	Valve
Mode	Design	Design
Active	☐	☐
Status	Complete	Complete
Design Limit	DC Backup	Weir Loading
Limiting Stage	1__Main TS	28__Main TS

11. Click the **Design** tab, then select the **Specs** page.
12. In the **Number of Flow Paths** cell, enter **3** for both Section_1 and Section_2.
13. Click the **Performance** tab, then select the **Results** page to see the dimensions and configuration of the trays for Section_1 and Section_2. Since Section_1 is sized as having the largest tray diameter, its tray section parameters should be recorded.
14. Confirm the following tray section parameters for Section_1.

Variable	Value
Section Diameter	5.639 m
Weir Height	0.0508 m
Tray Spacing	0.6096 m
Total Weir Length	13.31 m

The number of flow paths for the vapour is 3. The Actual Weir length is therefore the Total Weir Length recorded/3.

15. Calculate the Actual Weir length:

Variable	Value
Actual Weir Length (Total Weir Length/3)	4.44 m

16. Confirm the Maximum Pressure Drop/Tray and check the number of trays in the Main TS column. The Total Section Pressure drop is calculated by multiplying the number of trays by the Maximum Pressure Drop/Tray.

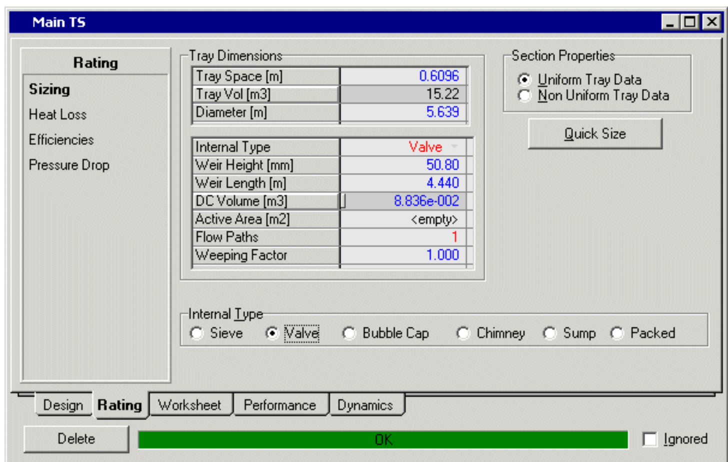
Variable	Value
Maximum Pressure Drop/Tray	0.86 kPa
Number of Trays	29
Total Section DeltaP	24.94 kPa

17. Close the Tray Sizing: Main TS and Available Utilities views.
18. Double-click on the Column T-100 icon in the PFD, then click the **Column Environment** button to enter the Column subflowsheet.
19. On the column PFD, double-click the Main TS Column icon to enter the Main TS property view.
20. Click the **Rating** tab, then select the **Sizing** page.

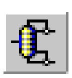
Be aware that the default units for each tray section parameter may not be consistent with the units provided in the tray sizing utility. You can select the units you want from the drop-down list that appears beside each input cell.

21. Enter the previous calculated values into the following tray section parameters:
    - Diameter 5.639m
    - Tray Spacing 0.6096m
    - Weir Height 0.0508m
    - Weir Length (Actual Weir Length) 4.44m
22. In the Internal Type group, select the **Valve** radio button.

Figure 2.157



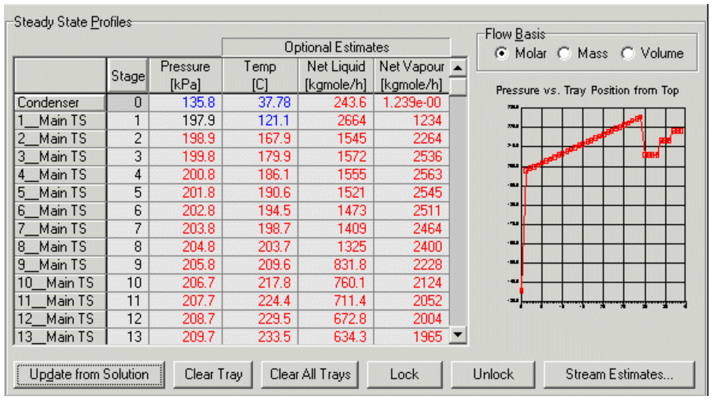
23. Close the Main TS property view.
24. Access the Column property view by clicking the **Column Runner** icon in the tool bar.



Column Runner icon

25. Click the **Parameters** tab, then select the **Profiles** page. Observe the steady state pressure profile across the column.

Figure 2.158



26. Record the top stage pressure (1_Main TS). Calculate the theoretical bottom stage pressure as follows:

$$\text{Bottom Stage Pressure} = \text{Top Stage Pressure} + \text{Total Section Pressure Drop} \quad (2.1)$$

Variable	Value
Top Stage Pressure	197.9 kPa
Total Section Pressure Drop	24.94 kPa
Bottom Stage Pressure	222.84 kPa

27. In the **Pressure** column of the Profiles group, specify a bottom stage pressure (29_Main TS) of 222.84 kPa.

Run Column Solver icon

28. Converge the Column sub-flowsheet by clicking the **Run Column Solver** icon in the tool bar.

29. Close the Column property view.

Side Stripper Tray Sizing

In this section, you will size the following side stripper operations using the tray sizing utility as described in the Column Tray Sizing section.

- Kero_SS
- Diesel_SS
- AGO_SS

1. From the **Tools** menu, select **Utilities**. The Utilities property view appears.
2. Double-click on the Tray Sizing utility. The Tray Sizing view appears.
3. In the **Name** field, change the name to **Kero_SS TS**.

4. Click the **Select TS** button. The Select Tray Section view appears.
5. From the Flowsheet list, select **T-100**, then select **Kero_SS** from the Object list. Click the **OK** button.
6. Click the **Auto Section** button. The Auto Section Information view appears.
7. Select the **Valve** radio button and click the **Next** button.
8. Click the **Complete AutoSection** button to calculate the Kero_SS TS tray sizing parameters.
9. Record the following tray section parameters available on the **Performance** tab in the **Results** page:

Variable	Kero_SS
Section Diameter	1.676 m
Weir Height	0.0508 m
Tray Spacing	0.6096 m
Total Weir Length	1.362 m
Number of Flow Paths	1
Actual Weir Length (calc)	1.362 m

10. Close the Kero_SS TS tray sizing utility.
11. Repeat steps #2-#8 to size the **Diesel_SS** and **AGO_SS** side strippers.
12. Click the **Performance** tab, select the **Results** page, then confirm that the following tray section parameters match the table below:

Variable	Diesel_SS	AGO_SS 1	AGO_SS 2
Section Diameter	1.676 m	1.067 m	0.6096 m
Weir Height	0.0508 m	0.0508 m	0.0508 m
Tray Spacing	0.6096 m	0.6096 m	0.6096 m
Total Weir Length	3.029 m	0.7038 m	0.5542 m
Number of Flow Paths	2	1	1
Actual Weir Length (calc)	1.515 m	0.7038 m	0.5542 m

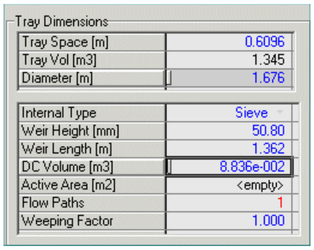
The pressure drop rating information found in the side stripper tray sizing utilities is not used to specify the pressure profile of the Side Stripper unit operations. Since there are only three trays in each side stripper, the pressure drop across the respective tray sections is small. Keeping the pressure profile across the side strippers constant does not greatly impact the transition from steady state mode to dynamics.

13. Close the Available Utilities view.

You should still be in the Column sub-flowsheet environment. If not, double-click the Column T-100 and then click the **Column Environment** button on the bottom of the Column property view.

14. In the PFD, double-click the Kero_SS side stripper icon to open its property view.
15. Click the **Rating** tab, then select the **Sizing** page.
16. Specify the following tray section parameters that were calculated in the previous table:
    - Section Diameter
    - Tray Spacing
    - Weir Height
    - Actual Weir Length

Figure 2.159



17. Close the Kero_SS property view.
18. Double-click the **Diesel_SS** icon, then specify the tray rating information using the table on the previous page. Close the property view when you are done.
19. Repeat the same procedure to specify the tray rating information for **AGO_SS**.
20. After the column has been specified with the tray rating information, converge the column by clicking the **Run Column Solver** icon in the toolbar.

Run Column Solver icon

21. Save the case as **DynTUT2-2.usc**.

Vessel Sizing

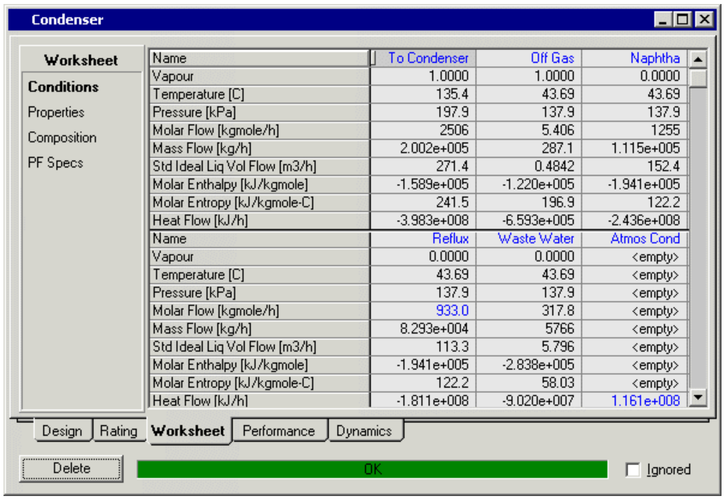
The Condenser and Kero_SS_Reb operations require proper sizing before they can operate effectively in dynamic mode. The volumes of these vessel operations are determined based on a 10 minute liquid residence time.

1. Double-click the Condenser icon on the PFD to open its property

view.

2. Click the **Worksheet** tab, then select the **Conditions** page.

Figure 2.160



3. On the **Conditions** page, confirm the following Liquid Volumetric Flow (Std Ideal Liq Vol Flow) of the following streams:

Liquid Volumetric Flow Rate (m3/h)	Value
Reflux	106.7
Naphtha	152.4
Waste Water	5.736
To Condenser	264.8

4. Calculate the vessel volume as follows, assuming a 50% liquid level residence volume and a 10 min. residence time:

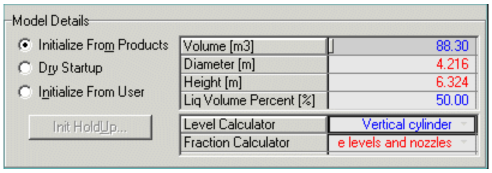
$$Vessel\ Volume = \frac{Total\ Liquid\ Exit\ Flow \times Residence\ \ Time}{0.5} \qquad (2.2)$$

The vessel volume calculated for the Condenser is **88.3 m**^{3}.

5. Click the **Dynamics** tab, then select the **Specs** page.

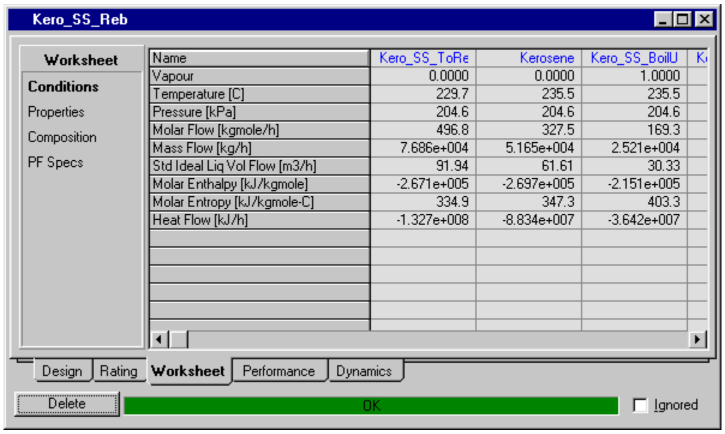
6. In the Model Details group, specify the vessel **Volume** as **88.3 m**^{3} and the Level Calculator as a Vertical Cylinder.

Figure 2.161



7. Close the Condenser property view.
8. In the PFD, double-click the **Kero_SS_Reb** icon to open its property view.
9. Click the **Worksheet** tab, then select the **Conditions** page.

Figure 2.162



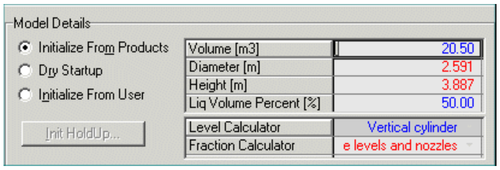
10. In the **Conditions** page, confirm that the Liquid Volumetric Flow (Std Ideal Liq Vol Flow) for Kerosene is 61.61 m^3/h.

    Assume a 10 minute of residence time and a 50% liquid level residence volume. The vessel volume calculated for the Kero_SS_Reb is **20.5 m**^{3}.

11. Click the **Dynamics** tab, then select the **Specs** page.

12. In the **Volume** cell, enter **20.5 m**^{3}. In the Level Calculator cell, select **Horizontal Cylinder** from the drop-down list.

Figure 2.163



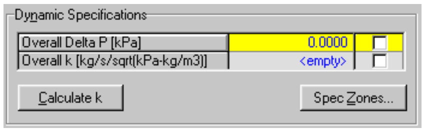
13. Close the Kero_SS_Reb property view.

Cooler Volume Sizing

UniSim Design assigns a default volume to each Cooler unit operation in the Column sub-flowsheet. In this section you will modify each pump around cooler to initialize with a default vessel volume.

1. Double-click the **PA_1_Cooler** operation in the PFD to open the property view.
2. Click the **Dynamics** tab, then select the **Specs** page.
3. In the Model Details group, click in the **Volume** cell, then press **DELETE**. The default volume of 0.10 m^3 appears.
4. In the Dynamic Specifications group, ensure that all the specification checkboxes are inactive. No dynamic specifications should be set for the pump around coolers.

Figure 2.164



5. Close the PA_1_Cooler view.
6. Repeat this process for the PA_2_Cooler and the PA_3_Cooler operations.
7. Save the case as **DynTUT2-3.usc**.

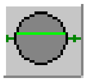
2.3.3 Adding Controller Operations

Controller operations can be added before or after the transition to dynamic mode. Key control loops are identified and controlled using

PID Controller logical operations. Although these controllers are not required to run the design in dynamic mode, they increase the realism of the model and provide more stability.

Adding a Level Controller

In this section you will add level controllers to the simulation flowsheet to control the levels of the condenser and reboiler.



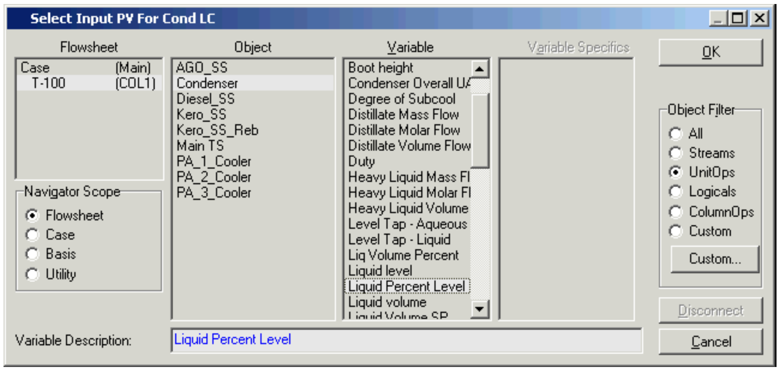
PID Controller icon

For more information regarding PID Controller, see **Section 12.4.4 - PID Controller** of the **UniSim Design Operations Guide**.

First you will install the Condenser controller.

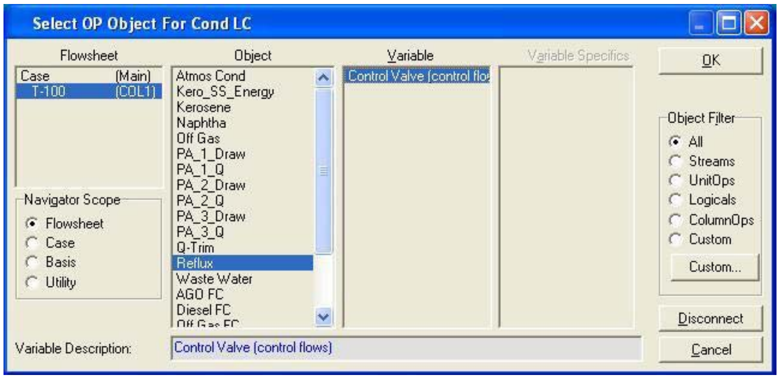
1. If the Object Palette is not visible, press **F4**.
2. In the Object Palette, click the **PID Controller** icon.
3. In the PFD, click near the Condenser operation. The controller icon, named IC-100, appears in the PFD.
4. Double-click the IC-100 icon to open the controller property view.
5. On the **Connections** tab, click in the **Name** field and change the name of the Controller to Cond LC.
6. In the Process Variable Source group, click the **Select PV** button, then select the information as shown in the figure below. Click the **OK** button when you are done.

Figure 2.165



7. In the Output Target Object group, click the **Select OP** button, then select the information as shown in the figure below. Click the **OK** button when you are finished.

Figure 2.166

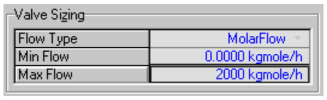


8. Click the **Parameters** tab, then select the **Configuration** page.
9. Supply the following for the **Configuration** page:

In this cell...	Enter...
Action	Direct
Kc	4
Ti	5 minutes
PV Minimum	0%
PV Maximum	100%

10. Click the **Control Valve** button. The FCV for Reflux view appears.
11. In the **Max Flow** cell of the Valve Sizing group, enter 2000 kgmole/h.

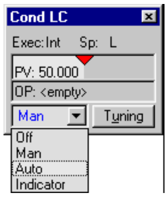
Figure 2.167



12. Close the FCV for Reflux view.
13. Click the **Face Plate** button. The face plate for Cond LC appears.

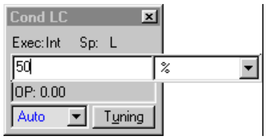
For more information regarding Face Plates, see **Section 12.13 - Controller Face Plate** in the **UniSim Design Operations Guide**.

Figure 2.168



14. Change the controller mode to Auto on the face plate by opening the drop-down list and selecting Auto.
15. Double-click the **PV** cell, then input the set point at 50%.

Figure 2.169



16. Close the Cond LC property view, but leave the face plate view open.

If you cannot locate a stream or operation in the Select Input for PV view, select the **All** radio button in the Object Filter group and look again.

17. Repeat the procedures you just learned to add a PID Controller operation which serves as the Kero_SS_Reb level controller. Specify the following:

Tab [Page]	In this cell...	Enter...
Connections	Name	Reb LC
	Process Variable Source	Kero_SS_Reb, Liq Percent Level
	Output Target Object	Kero_SS_Draw
Parameters [Configuration]	Action	Reverse
	Kc	1
	Ti	5 minutes
	PV Minimum	0%
	PV Maximum	100%

18. Click the **Control Valve** button. The FCV for Kero_SS_Draw view appears.
19. In the Valve Sizing group, enter the following

In this cell...	Enter...
Flow Type	MolarFlow
Minimum Flow	0 kgmole/h
Maximum Flow	1000 kgmole/h

20. Close the FCV for Kero_SS_Draw view.
21. Click the **Face Plate** button. Change the controller mode to Auto on the face plate, then input a set point of 50%. Leave the face plate view open.
22. Close the Reb LC property view.

Adding a Flow Controller

In this section you will add flow controllers to the product streams of

the column. These controllers ensure that sufficient material is leaving the column.

1. Click the PID Controller icon in the Object Palette, then click in the PFD near the Off Gas stream. The controller icon appears.
2. Double-click the controller icon to access the property view. Specify the following details:

Tab [Page]	In this cell...	Enter...
Connections	Name	Off Gas FC
	Process Variable Source	Off Gas, Molar Flow
	Output Target Object	Atmos Cond
Parameters [Configuration]3	Action	Direct
	Kc	0.01
	Ti	5 minutes
	PV Minimum	0 kgmole/h
	PV Maximum	100 kgmole/h

3. Click the **Control Valve** button. The FCV for Atmos Cond view appears.
4. In the Duty Source group, ensure that the **Direct Q** radio button is selected.
5. In the Direct Q group, enter the following details:

In this cell...	Enter...
Minimum Available	0 kJ/h
Maximum Available	2 x 10^8 kJ/h

6. Close the FCV for Atmos Cond view.
7. Click the **Face Plate** button. The Off Gas FC face plate view appears. Change the controller mode to Auto, then input a set point of **5** kgmole/h.
8. Close the Off Gas FC property view, but leave the face plate view open.
9. In the Object Palette, click the **PID Controller** icon, then click in the PFD near the Diesel stream. The controller icon appears in the PFD.
10. Double-click the controller icon to access the property view. then specify the following details:

Tab [Page]	In this cell...	Enter...
Connections	Name	Diesel FC
	Process Variable Source	Diesel, Liq Vol Flow@Std Cond
	Output Target Object	Diesel_SS_Draw

Tab [Page]	In this cell...	Enter...
Parameters [Configuration]	Action	Reverse
	Kc	1
	Ti	5 minutes
	PV Minimum	0 m3/h
	PV Maximum	250 m3/h

11. Click the **Control Valve** button. The FCV for Diesel_SS_Draw view appears.
12. In the Valve Sizing group, enter the following details:

In this cell...	Enter...
Flow Type	MolarFlow
Minimum Flow	0 kgmole/h
Maximum Flow	1200 kgmole/h

13. Close the FCV for Diesel_SS_Draw view.
14. Click the **Face Plate** button. The Diesel FC face plate view appears. Change the controller mode to Auto and input a set point of 127.5 m3/h.
15. Close the property view, but leave the face plate view open.
16. Click the **PID Controller** icon in the Object Palette, then click near the AGO stream on the PFD. The controller icon appears.
17. Double-click the controller icon, then specify the following details:

Tab [Page]	In this cell...	Enter...
Connections	Name	AGO FC
	Process Variable Source	AGO, Liq Vol Flow@Std Cond
	Output Target Object	AGO_SS_Draw
Parameters [Configuration]	Action	Reverse
	Kc	0.7
	Ti	3 minutes
	PV Minimum	0 m3/h
	PV Maximum	60 m3/h

18. Click the **Control Valve** button. The FCV for AGO_SS_Draw view appears.
19. In the Valve Sizing group, enter the following details:

In this cell...	Enter...
Flow Type	MolarFlow
Minimum Flow	0 kgmole/h
Maximum Flow	250 kgmole/h

20. Close the FCV for AGO_SS_Draw view.

21. Click the **Face Plate** button. The AGO FC face plate view appears. Change the controller mode to Auto and input a set point of 29.8 m3/h.
22. Close the property view, but leave the face plate view open.
23. Save the case as **DynTUT2-4.usc**.

2.3.4 Adding Pressure-Flow Specifications

Before integration can begin in UniSim Design, the degrees of freedom for the flowsheet must be reduced to zero by setting the pressure-flow specifications. Normally, you make one pressure-flow specification per flowsheet boundary stream, however, there are exceptions to the rule. One extra pressure flow specification is required for every condenser or side stripper unit operation attached to the main column. This rule applies only if there are no pieces of equipment attached to the reflux stream of the condenser or the draw stream of the side strippers. Without other pieces of equipment (i.e., pumps, coolers, valves) to define the pressure flow relation of these streams, they must be specified with a flow specification.

Pressure-flow specifications for this case will be added to the following boundary streams:

- Atm Feed
- Main Steam
- AGO Steam
- Diesel Steam
- Off Gas
- Waste Water
- Naphtha
- Kerosene
- Diesel
- AGO
- Residue

For more information regarding Pressure Flow specifications in Column unit operations see **Chapter 8 - Column** in **UniSim Design Operations Guide**.

This simplified column has all the feed streams specified with a flow specification. The Off Gas stream has a pressure specification which defines the pressure of the condenser and consequently the entire column. The liquid exit streams of the column and the side stripper operations require pressure specifications since there are no attached pieces of equipment in these streams. All the other exit streams associated with the column require flow specifications.

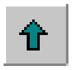
The following pump around streams require flow specifications since both the Pressure Flow and the Delta P specifications are not set for the

pump around coolers.

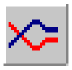
- PA_1_Draw
- PA_2_Draw
- PA_3_Draw

The following streams have their flow specifications defined by PID Controller operations.

- Reflux
- Kero_SS_Draw
- Diesel_SS_Draw
- AGO_SS_Draw



Enter Parent Simulation Environment icon

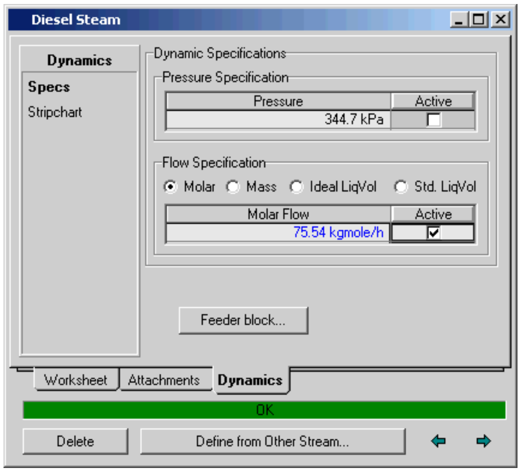


Dynamic Mode icon

1. Enter the Main Flowsheet environment. Close the column property view if it is still open.
2. Switch to dynamic mode by clicking the **Dynamic Mode** icon. When asked if you want to allow dynamics assistant to identify items which are needed to be addressed before proceeding into dynamics, click the **No** button.

   Every material stream in the Main Flowsheet requires either a pressure or flow specification.
3. Double-click the Diesel Steam icon to enter its property view.
4. Click the **Dynamics** tab, then select the **Specs** page.
5. In the Pressure Specification group, clear the **Active** checkbox.
6. In the Flow Specification group, select the **Molar** radio button, then activate the **Active** checkbox.
7. In the **Molar Flow** cell, enter 75.54 kgmole/h if required.

Figure 2.170



Once a pressure or flow specification has been made active, the stream value turns blue and can be modified.

Set the following pressure or flow specifications for the following

streams in the Main Flowsheet.

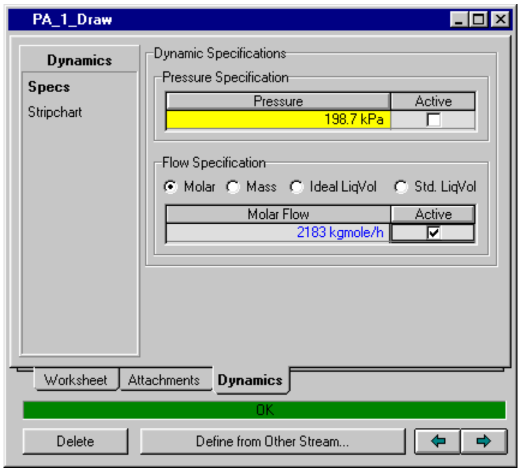
Material Stream	Pressure Specification	Flow Specification	Value
Atm Feed	Inactive	Molar Flow, Active	2826 kgmole/h
Main Steam	Inactive	Molar Flow, Active	188.8 kgmole/h
AGO Steam	Inactive	Molar Flow, Active	62.95 kgmole/h
Off Gas	Active	Inactive	135.8 kPa
Waste Water	Inactive	Molar Flow, Active	317.8 kgmole/h
Naphtha	Inactive	Ideal LiqVol, Active	152.4 m3/h
Kerosene	Inactive	Ideal LiqVol, Active	61.61 m3/h
Diesel	Active	Inactive	211.4 kPa
AGO	Active	Inactive	215.6 kPa
Residue	Active	Inactive	221.6 kPa

8. Use the Object Navigator to enter the Column subflowsheet environment. Click the **Object Navigator** icon in the tool bar. The Object Navigator view appears. In the Flowsheets group, double-click T-100.

   Every material stream in the column environment also requires either a pressure or flow specification. Use the following procedure to set a pressure-flow specification for the PA_1_Draw stream.

9. In the PFD, double-click the PA_1_Draw stream icon to open the property view.
10. Click the **Dynamics** tab, then select the **Specs** page.
11. In the Flow Specification group, select the **Molar** radio button, then activate the **Active** checkbox.

Figure 2.171

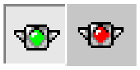


12. Close the PA_1_Draw property view.

13. Activate the following flow specifications for the following streams in the Column sub-flowsheet.

Material Stream	Pressure-Flow Specification	Value
PA_2_Draw	Molar Flow	830.2 kgmole/h
PA_3_Draw	Molar Flow	648.0 kgmole/h
Reflux	Molar Flow	879.7 kgmole/h
Kero_SS_Draw	Molar Flow	426.6 kgmole/h
Diesel_SS_Draw	Molar Flow	616.8 kgmole/h
AGO_SS_Draw	Molar Flow	124.8 kgmole/h

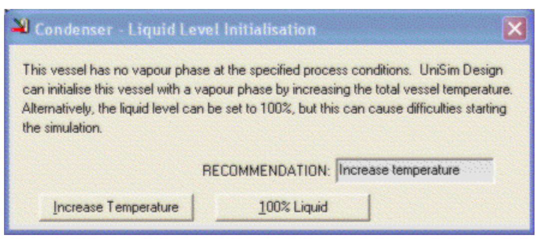
14. Save the case as **DynTUT2-5.usc**.
15. Close all the views except the face plates.
16. To arrange the face plates, select the **Arrange Desktop** command from the **Windows** menu.


Start Integrator icon

17. The integrator can be run at this point. Click the **Start Integrator** icon. When you are given the option to run dynamic assistant, select **No**.

    When the integrator initially runs, UniSim Design detects that no vapour phase exists in the Condenser at the specified process conditions. It displays the following message:

Figure 2.172



    UniSim Design recommends that you increase the temperature setting to create a vapour phase. You can also create a non-equilibrium vapour phase or set the liquid level to be 100%. For the sake of this example, select the default recommendation.

18. Click the **Increase Temperature** button.
19. Let the integrator run for few minutes so all the values can propagate through the column. Observe the value changes on the face plate view.
20. To stop the integrator, click the **Stop Integrator** icon.

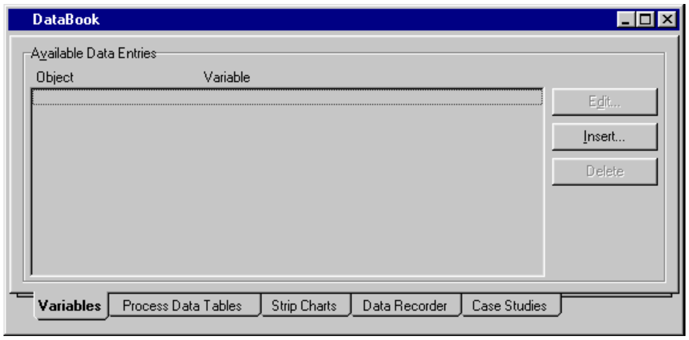
2.3.5 Monitoring in Dynamics

Now that the model is ready to run in dynamic mode, the next step is to

install a strip chart to monitor the general trends of key variables. The following is a general procedure for installing strip charts in UniSim Design.

1. Open the Databook by using the hot key combination **CTRL D**.

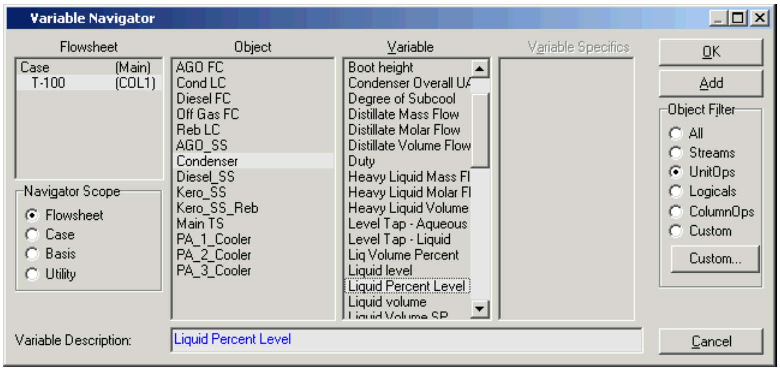
Figure 2.173



The Variable Navigator is used extensively in UniSim Design 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.

2. On the **Variables** tab, click the **Insert** button. The Variable Navigator view appears.
3. In the Flowsheet list, select the Column T-100.
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 the Condenser. The Variable list available for the column appears to the right of the Object list.
6. In the Variable list, select Liquid Percent Level.

Figure 2.174



7. Click the **OK** button. The variable now appears in the Databook.

If you can't find an Object in the Variable Navigator view, select the **All** radio button in the Object Filter group, then select Case (Main) in the Flowsheet group. All operations and streams for the design will appear in the Object list.

8. Add the following variables to the Databook. If you select the top variable in the list of Available Data Entries before inserting a new variable, the new variable will always be added to the top of the list.

Object	Variable
Kero_SS_Reb	Liquid Percent Level
Off Gas	Molar Flow
Condenser	Vessel Temperature

The next task is to create a Strip Chart to monitor the dynamics behaviour of the selected variables.

9. Click the **Strip Charts** tab in the Databook view.
10. Click the **Add** button. UniSim Design creates a new Strip Chart with the name DataLogger1.
11. Click in the blank **Active** checkbox beside the Condenser/Liquid Percent Level variable.

3 Chemicals Tutorial

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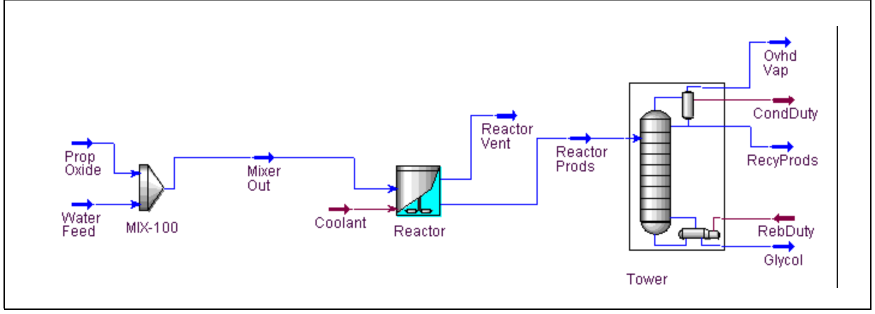
3.1 Introduction

The complete case for this tutorial has been pre-built and is located in the file **TUTOR3.usc** in your **UniSim Design\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 UniSim Design 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 UniSim Design interface will be utilized to illustrate the flexibility available to you.

Before proceeding, you should have read Chapter A - UniSim Design Tutorials which precedes the tutorials in this guide.

3.2 Steady State Simulation

The simulation will be built using these basic steps:

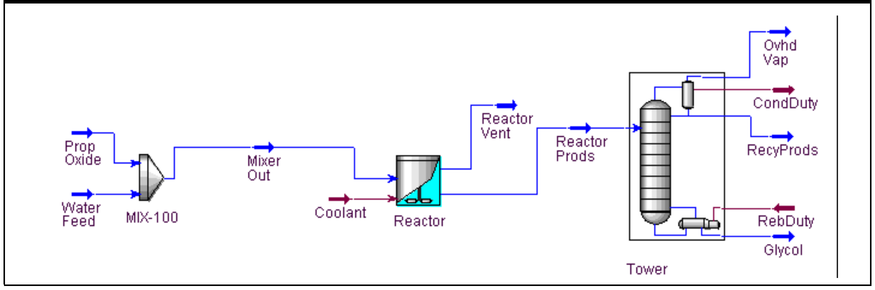
1. Select the components.
2. Choose a property package.
3. Create a fluid package.
4. Define the reaction.
5. Create and specify the feed streams.
6. Install and define the Mixer and Reactor.
7. Install and define the Distillation Column.

3.2.1 Process Description

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.

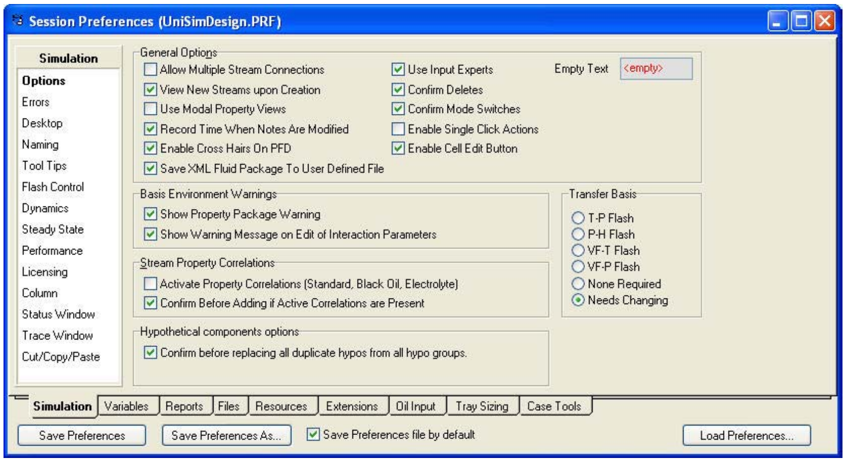
3.2.2 Setting Your Session Preferences

Start UniSim Design. 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. UniSim Design 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 UniSim Design Field set, then customize it.

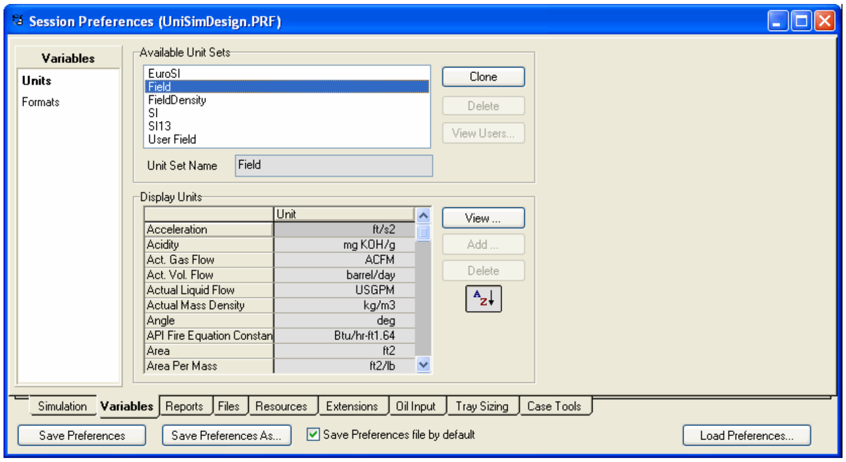
1. In the Available Units Sets list, select **Field**.

   The default unit for **Liq. Vol. Flow** is **barrel/day**; next you will

The default Preference file is named **unisimdesign R*.prf**. When you modify any of the preferences, you can save the changes in a new Preference file by clicking the **Save Preferences As...** button. UniSim Design 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.

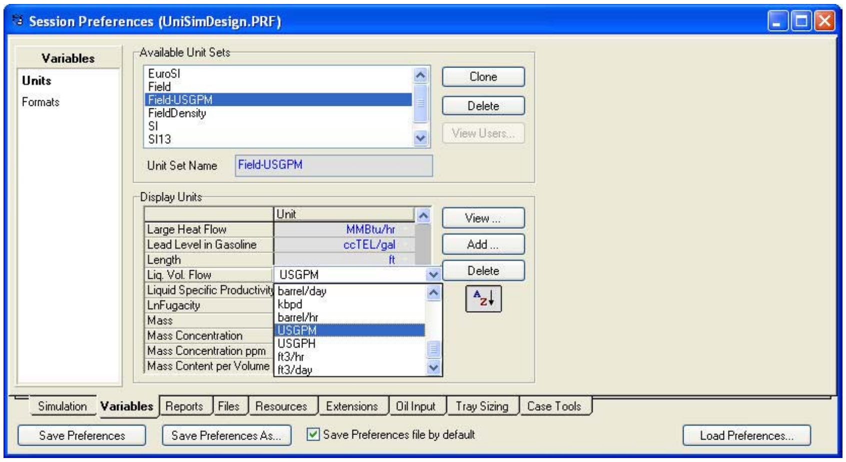
change the **Liq. Vol. Flow** units to **USGPM**.

Figure 3.4



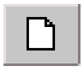
2. Click the **Clone** button. A new unit set named **NewUser** appears in the Available Unit Sets list.
3. In the **Unit Set Name** field, change the name to Field-USGPM. You can now change the units for any variable associated with this new unit set.
4. Find the **Liq. Vol. Flow** cell. Click in the **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. The new unit set is now defined. Close the Session Preferences view.

3.2.3 Building the Simulation

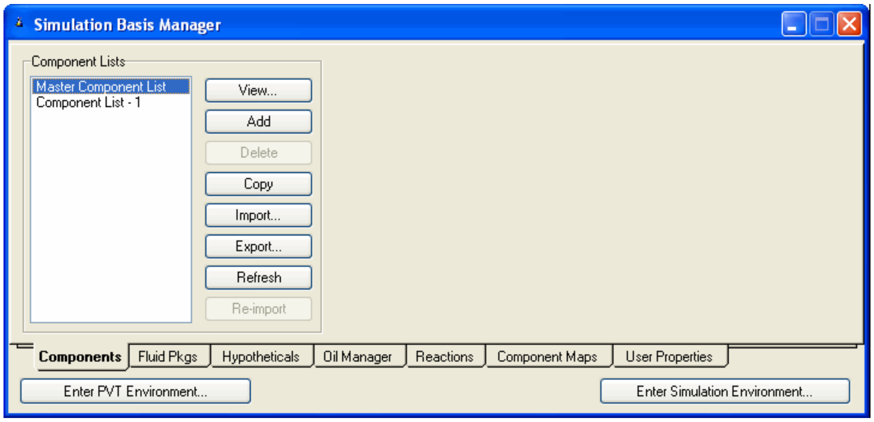


New Case Icon

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



UniSim Design 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 select the components. Then a Fluid Package will be created. A Fluid Package, at minimum, contains the components and property method that UniSim Design 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.

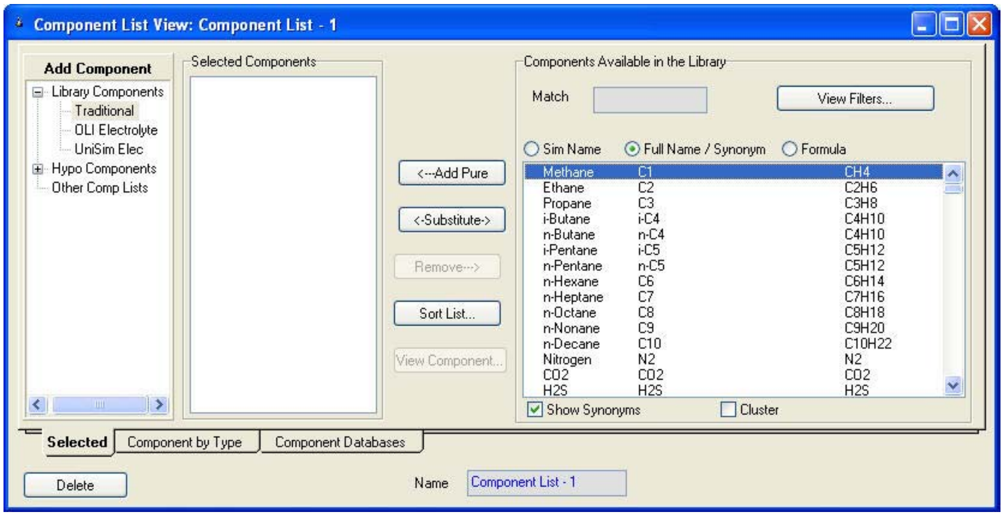
Selecting Components

Now that you have created a new case, your next task is to select the components.

1. On the **Components** tab of the Simulation Basis Manager view, click the **Add** button in the Component Lists group. The Component

List view appears.

Figure 3.7



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

Feature	Description
Sim Name	The name appearing within the simulation.
Full Name/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.

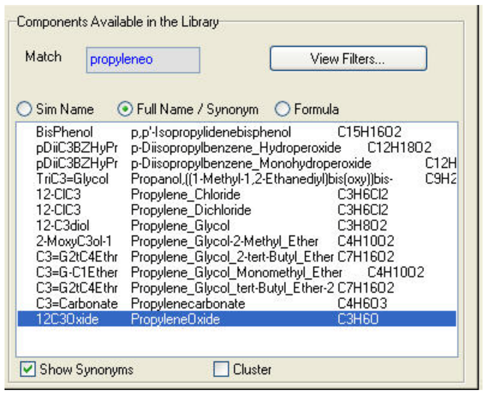
Based on the selected radio button, UniSim Design locates the component(s) that best matches the information you type in the **Match** field.

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 **Full Name / Synonym** radio button is selected and the **Show Synonyms** checkbox is checked.

3. In the **Match** field, start typing **propyleneoxide, as one word**. UniSim Design filters the list as you type, displaying only those components that match your input.

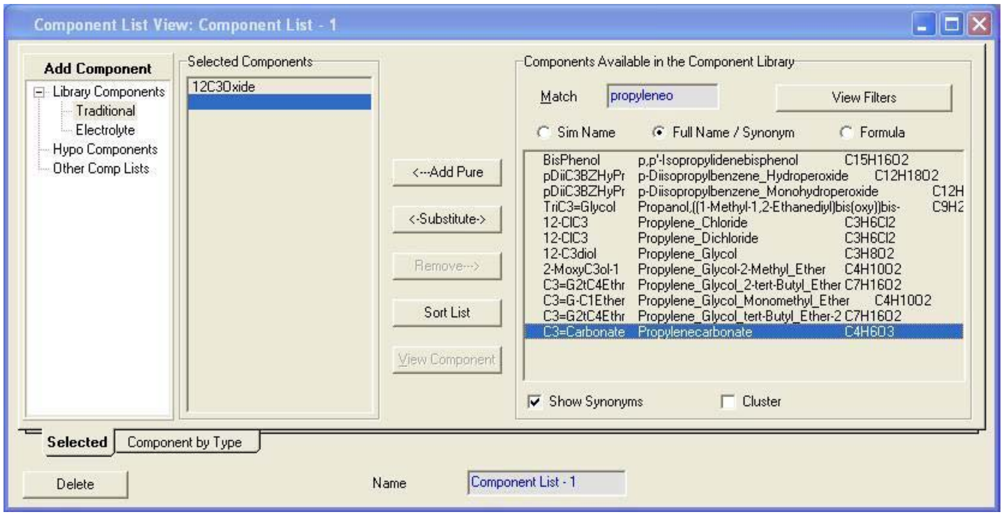
Figure 3.8



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**.

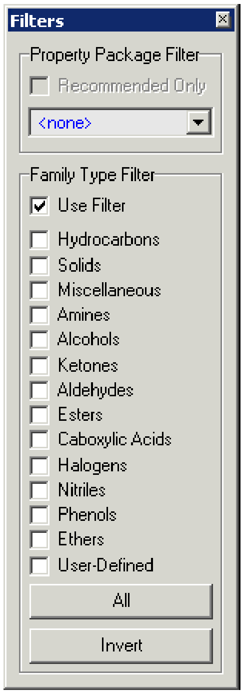
The component now appears in the **Selected Components list**.

Figure 3.9



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

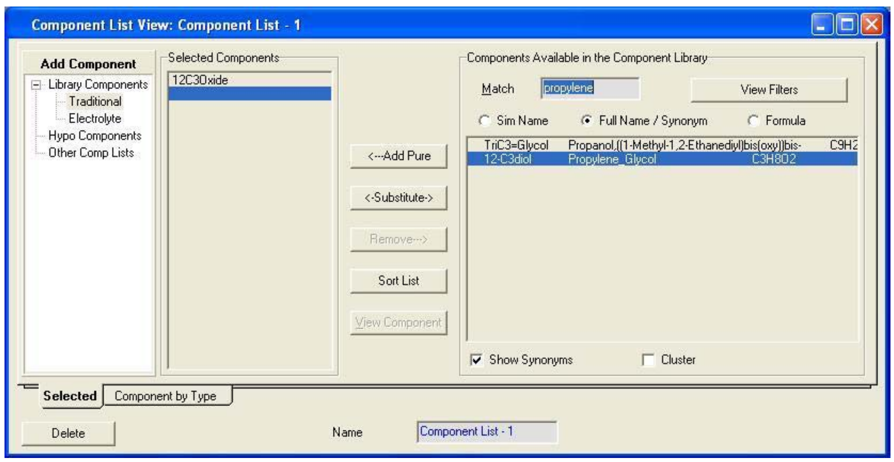
Next, you will add Propylene Glycol to the component list using the



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**. UniSim Design filters as you type, displaying only the alcohols that match your input.

Figure 3.10



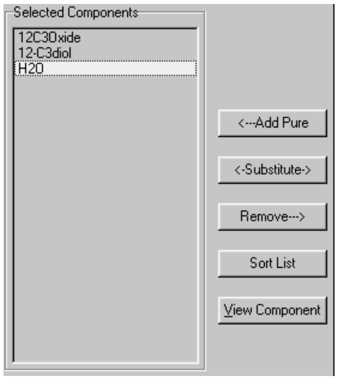
10. When **Propylene Glycol** is selected in the list, press the **ENTER** key to add it to the Selected Components list.

    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**.

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

15. The final component list appears below.

Figure 3.11

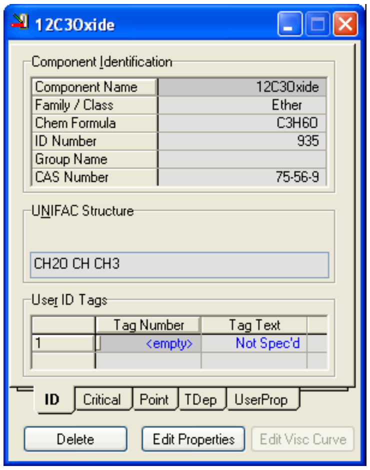


Viewing Component Properties

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

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

Figure 3.12



Refer to **Chapter 3 - Hypotheticals** in the **UniSim Design Simulation Basis Guide** for more information on cloning library components.

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, UniSim Design allows you to clone a library component into a Hypothetical component, which can then be modified as desired.

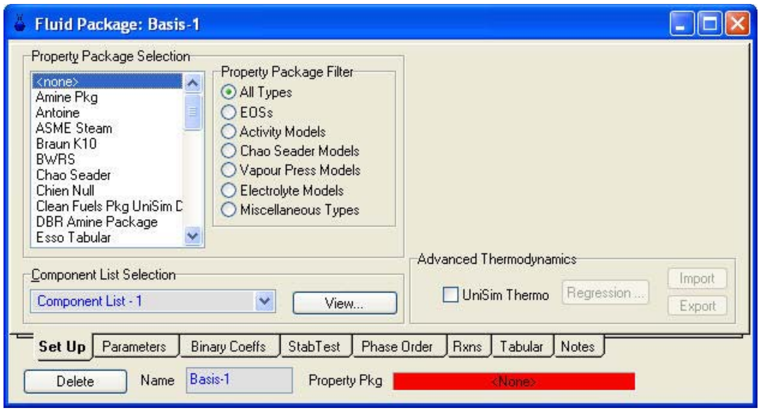
3. Close the individual component view, then close the Component List View to return to the Simulation Basis Manager.

Creating a Fluid Package

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.

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

Figure 3.13



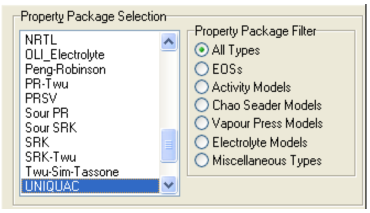
UniSim Design has created a Fluid Package with the default name **Basis-1**. You can change the name of this fluid package by typing a new name in the **Name** cell at the bottom of the view.

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 UniSim Design 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 3.14



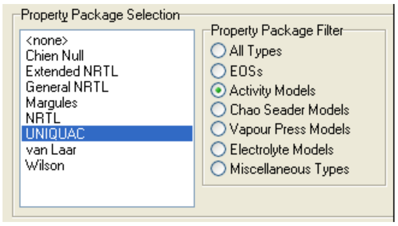
The **Property Pkg** indicator bar at the bottom of the view now

indicates **UNIQUAC** is the current property package for this Fluid Package.

Figure 3.15

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

Figure 3.16



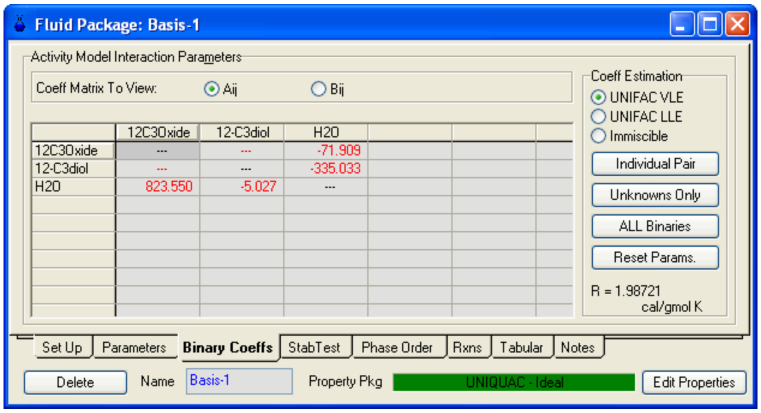
In the Component List Selection drop-down list, UniSim Design filters to the library components to include only those appropriate for the selected Property Package. In this case, Component List - 1 is selected as it is the only list you have created.

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



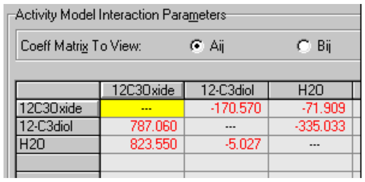
In the Activity Model Interaction Parameters group, the Aij interaction table appears by default. UniSim Design automatically inserts the coefficients for any component pairs for which library data is available. You can change any of the values provided by UniSim Design if you have data of your own.

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 UniSim Design's 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. UniSim Design provides values for the unknown pair. The final Activity Model Interaction Parameters table for the **Aij** coefficients appears below.

Figure 3.18



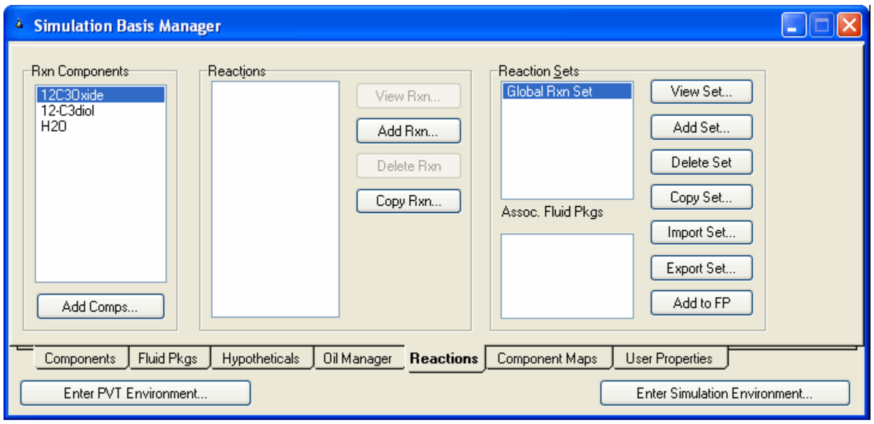
4. To view the Bij coefficient table, select the **Bij** radio button. For this example, all the Bij coefficients will be left at the default value of zero.

3.2.4 Defining the Reaction

Home View Icon

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

Figure 3.19



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.

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

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

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 - Building the Simulation** for more information.

Creating the Reaction

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

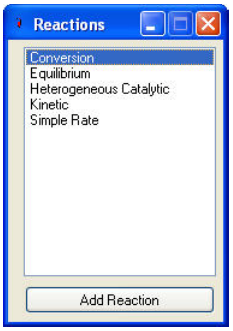
On the Stoichiometry tab, you can specify which of the Rxn Components are involved in the particular reaction as well as the stoichiometry and the reaction order.

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.

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

   The Reactions view appears.

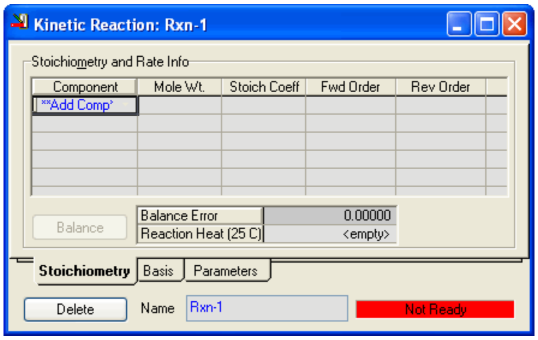
Figure 3.20



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.

Figure 3.21



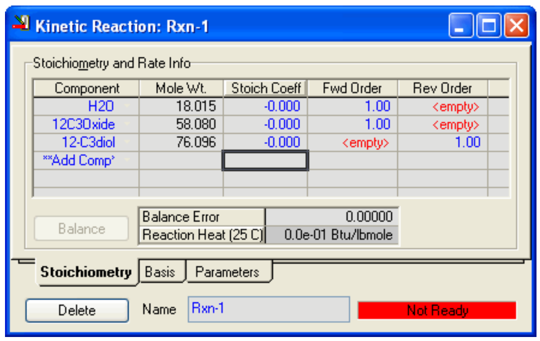
3. In the **Component** column, click in the cell labeled ****Add Comp****.
4. Select **Water** as a reaction component by doing **one** of the following:
   - Open the drop-down list and select H2O from the list of available reaction components.
   - Type H2O. UniSim Design filters as you type, searching 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



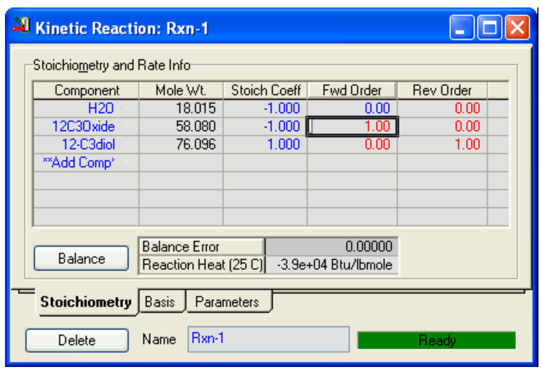
Once the stoichiometric coefficients are supplied, the **Balance Error** cell will show 0 (zero), indicating that the reaction is mass balanced. UniSim Design will also calculate and display the heat of reaction in the **Reaction Heat** cell. In this case, the **Reaction Heat** is negative, indicating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

UniSim Design 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.

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

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.

Figure 3.23



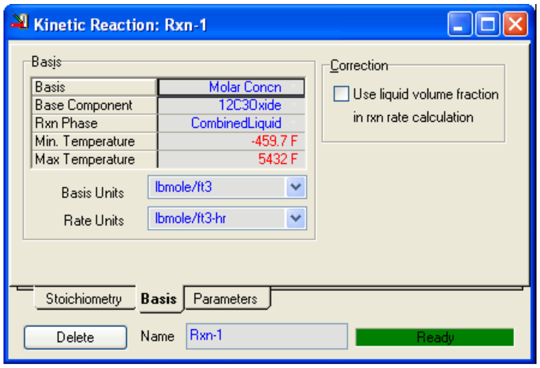
The next task is to define the reaction basis.

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, UniSim Design 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 UniSim Design 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

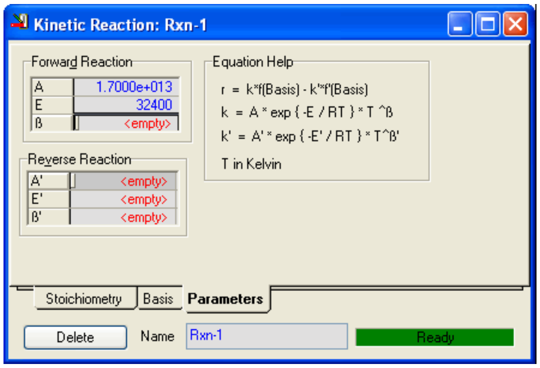


The **Min. Temperature**, **Max. Temperature**, **Basis Units,** and **Rate Units** are acceptable at their default values.

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

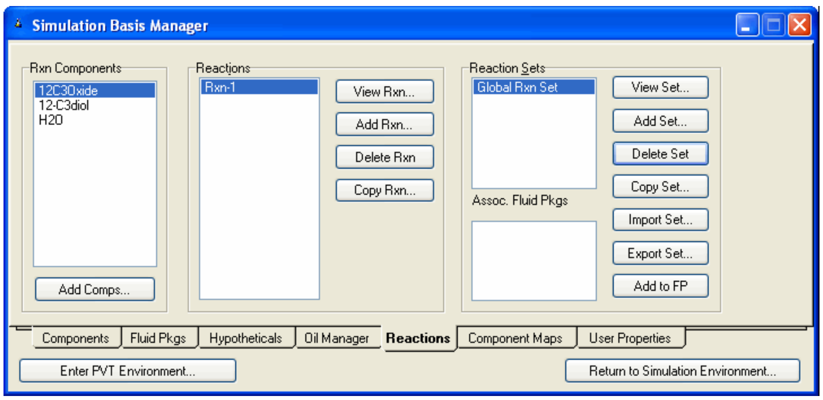


18. Close both the **Kinetic Reaction** property view and the **Reactions** view.

19. Click the **Home View** 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.

Home View Icon

Figure 3.26



The next task is to create a reaction set that will contain the new reaction. In the Reaction Sets list, UniSim Design 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

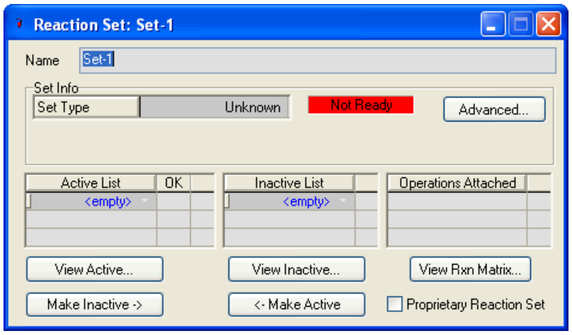
The same reaction(s) can be in multiple Reaction Sets.

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

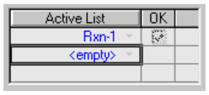


2. In the **Active List,** click in the cell labeled **<empty>**.
3. Open the drop-down list and select **Rxn-1**.

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.

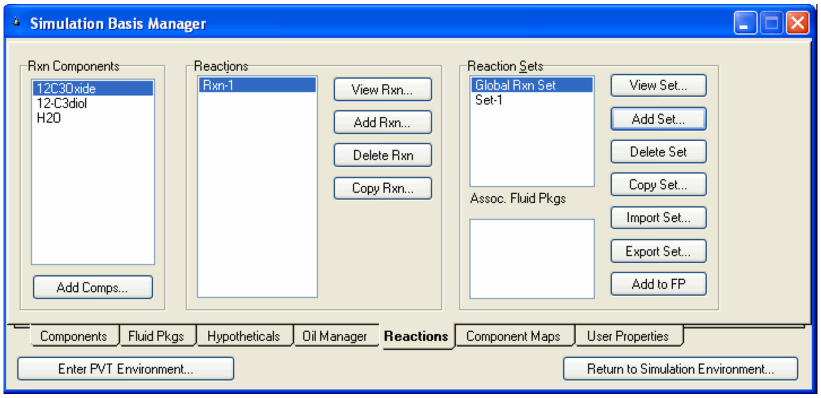
A checkbox labeled **OK** automatically appears next to the reaction in the **Active List**. The reaction set status bar changes from **Not Ready** to **Ready**, indicating that the new reaction set is complete.

Figure 3.28



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 3.29



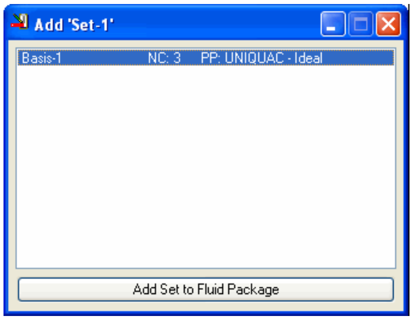
Making the Reaction Set Available to the Fluid Package

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.

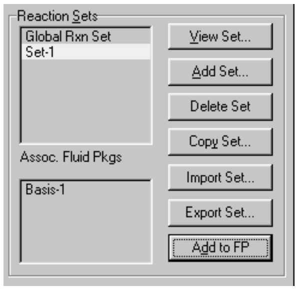
   This view prompts you to select the Fluid Package to which you would like to add the reaction set. In this example, there is only one Fluid Package, **Basis-1**.

Figure 3.30



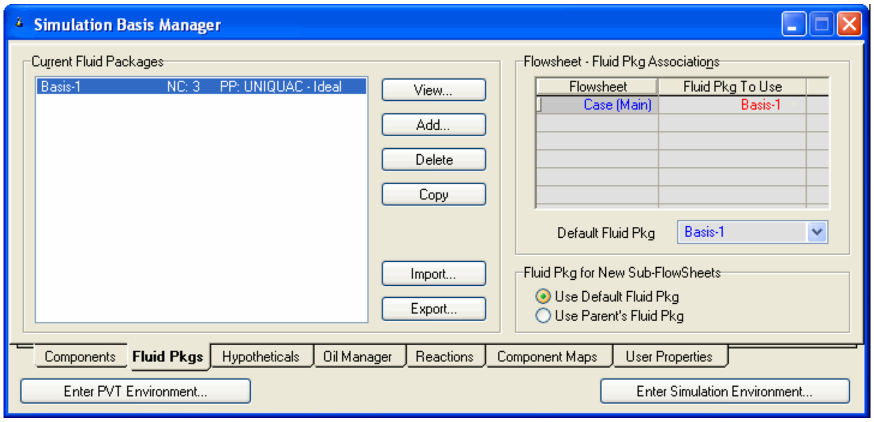
3. Select **Basis-1**, then click the **Add Set to Fluid Package** button.

Figure 3.31



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

Figure 3.32

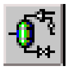


The list of **Current Fluid Packages** displays the new Fluid Package, **Basis-1**, showing the number of components (NC) and property package (PP). The new Fluid Package is assigned by default to the Main Simulation, as shown in the **Flowsheet - Fluid Pkg Associations** group. Now that the Basis is 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

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

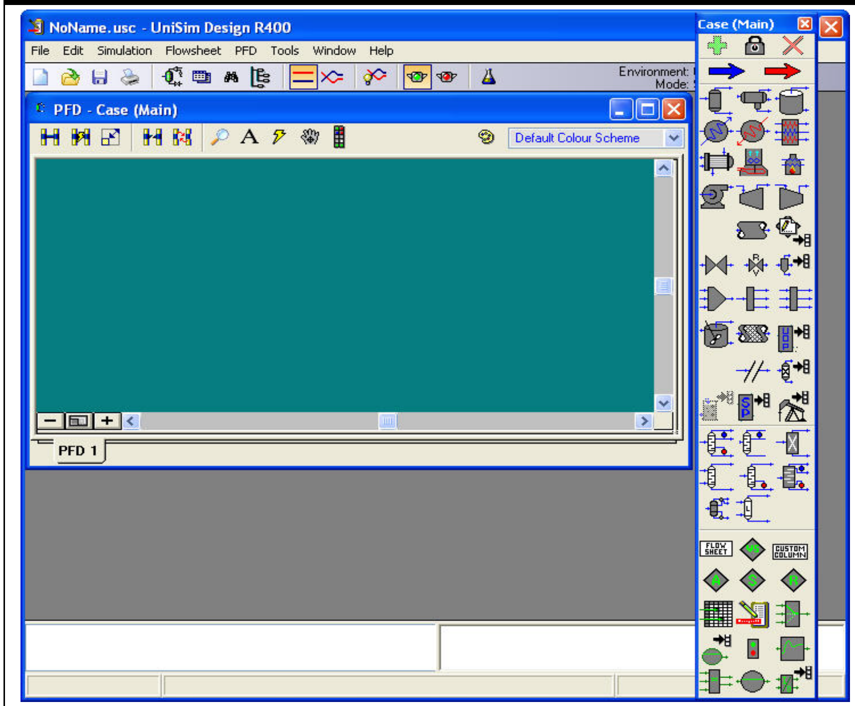
- Click the **Enter Simulation Environment** button on the Simulation Basis Manager.
- Click the **Enter Simulation Environment** icon on the toolbar.



Enter Simulation Environment Icon

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 tutorial, the initial Home View is the Workbook.

Figure 3.33



There are several things to note about the Main Simulation environment.

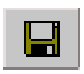
- In the upper right corner, the Environment has changed from Basis to Case (Main).

- 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.

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

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.

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



Save Icon

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

   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 **UniSim Design** directory.
2. In the **File Name** cell type a name for the case, for example **GLYCOL**. You do not have to enter the **.usc** extension; UniSim Design automatically adds it for you.

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

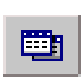
3. Once you have entered a file name, press the **ENTER** key or the **Save** button.

   UniSim Design 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.

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

1. Click the **Workbook** icon on the toolbar to make the **Workbook**

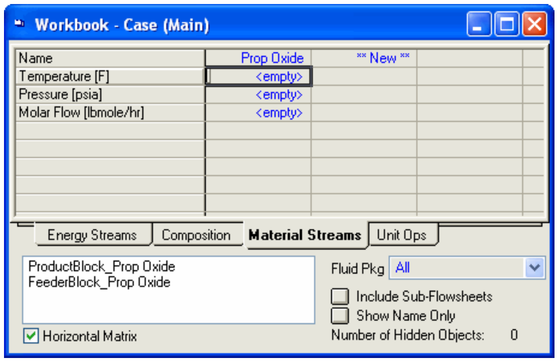
active.

2. On the **Material Streams** tab, click in the **New** cell in the Name row.

UniSim Design accepts blank spaces within a stream or operation name.

3. Type the new stream name Prop Oxide, then press **ENTER**. UniSim Design automatically creates the new stream.

Figure 3.34

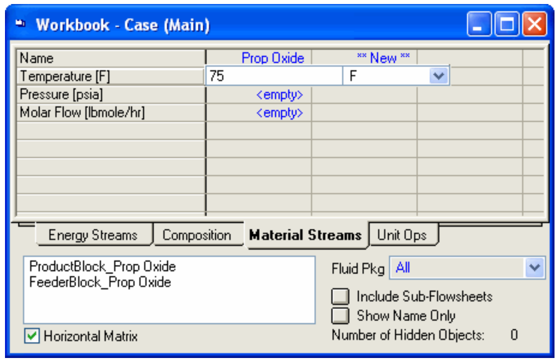


When you pressed **ENTER** after typing in the stream name, UniSim Design automatically advanced the active cell down one cell, to Vapour Fraction.

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, UniSim Design displays the default units for temperature, in this case **F**.

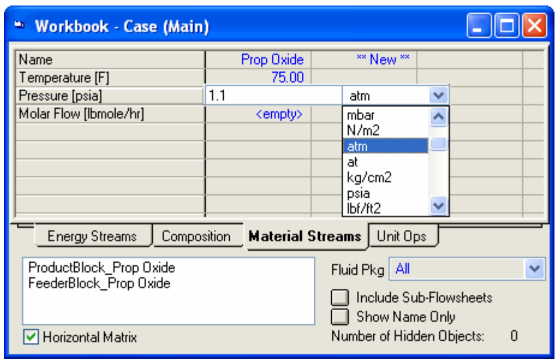
Figure 3.35



6. Since this is the correct unit, press **ENTER**. UniSim Design accepts the temperature.
7. You are now in the **Pressure** cell for Prop Oxide.

   If you know the stream pressure in another unit besides the default of psia, UniSim Design 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 **SPACE BAR** or click on . Begin typing '**atm'**. UniSim Design will match your input to locate the unit of your choice.

Figure 3.36



10. Once atm is selected in the list, press the **ENTER** key, and UniSim Design 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. **Enter 150 lbmole/hr** in the **Molar Flow** cell for **Prop Oxide, then press ENTER**.

Providing Compositional Input

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

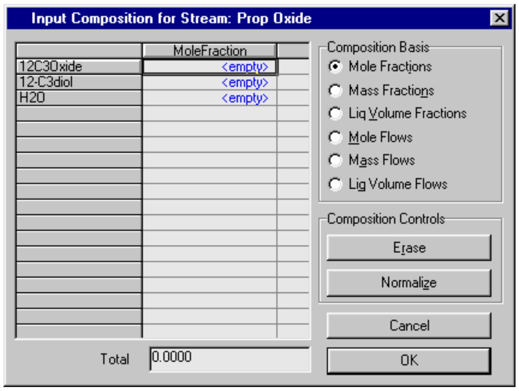
The Input Composition for Stream view is Modal, indicated by the thick border and the absence of the **Minimize/Maximize** buttons in the upper right corner. When a Modal view is visible, you will not be able to move outside the view until you finish with it, by clicking either the **Cancel** or **OK**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

1. 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 3.37



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

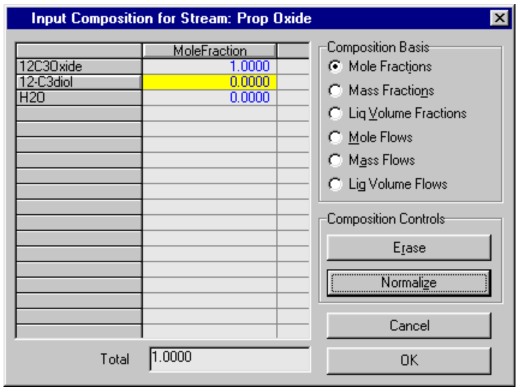
Features	Description
Composition Basis Radio Buttons	You can input the stream composition in some fractional basis other than Mole Fraction, or by component flows, by selecting the appropriate radio button before providing your input.
Normalizing	The Normalizing feature is useful when you know the relative 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. UniSim Design 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 UniSim Design forces the other component fractions to zero.

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

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

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

Figure 3.38

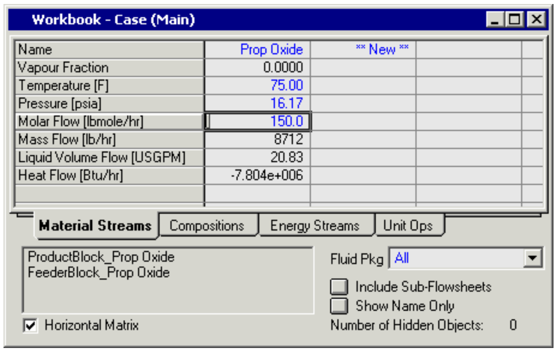


6. Click the **OK** button. UniSim Design accepts the composition. The stream specification is now complete, so UniSim Design will flash it at the conditions given to determine the remaining properties.

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

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

Figure 3.39



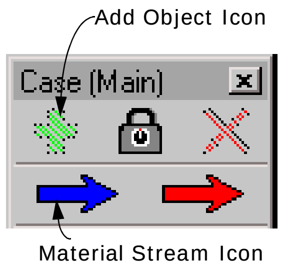
Adding Another Stream

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

1. 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.

Figure 3.40



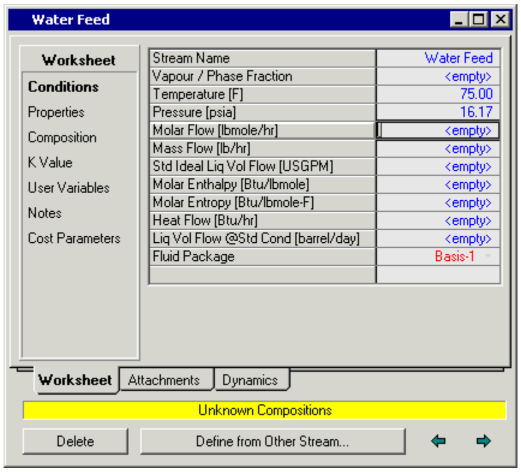
A new stream appears in the Workbook and is named according to the **Auto Naming** setting in your Session **Preferences settings**. The default setting names new material streams with numbers, starting at **1** (and energy streams starting at **Q-100**).

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

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

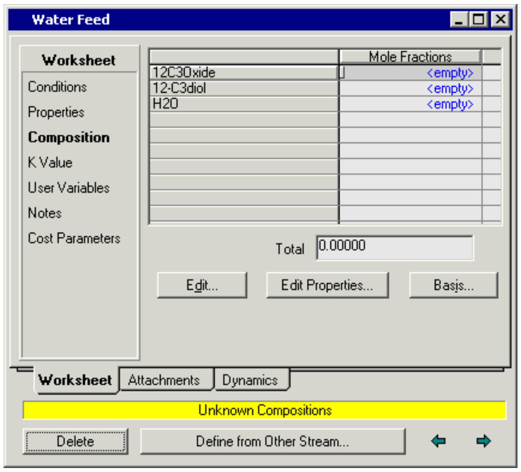
2. In the **Stream Name** cell, change the name to **Water Feed**.
3. In the **Temperature** cell, enter 75°F.
4. In the **Pressure** cell, enter **16.17 psia**.

Figure 3.41



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

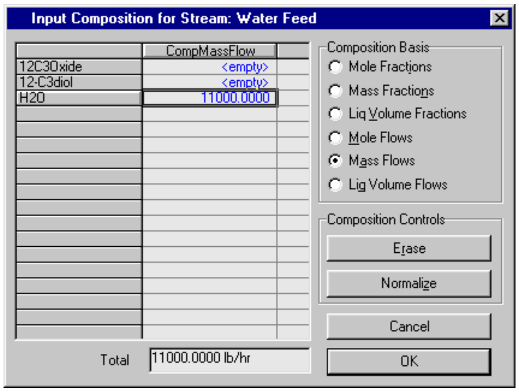
Figure 3.42



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

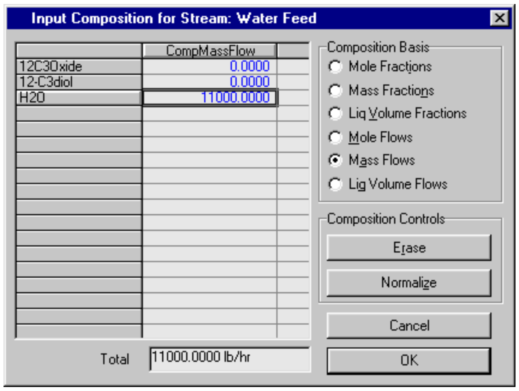
6. Click the **Edit** button near the bottom of the Composition page. The Input Composition for Stream view appears.
7. In the Composition Basis group, change the **basis** to **Mass Flows** by selecting the appropriate radio button, or by pressing **ALT a**.
8. In the **CompMassFlow** cell for **H2O**,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

Figure 3.43



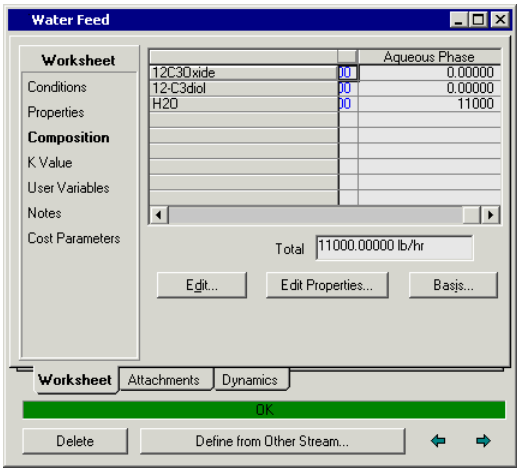
9. Since this stream has no other components, click the **OK** button. The other component mass flows are forced to zero.

Figure 3.44



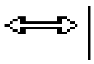
UniSim Design performs a flash calculation to determine the unknown properties of Water Feed, and the status bar displays a green OK message. Use the horizontal scroll bar in the table to view the compositions of each phase.

Figure 3.45



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

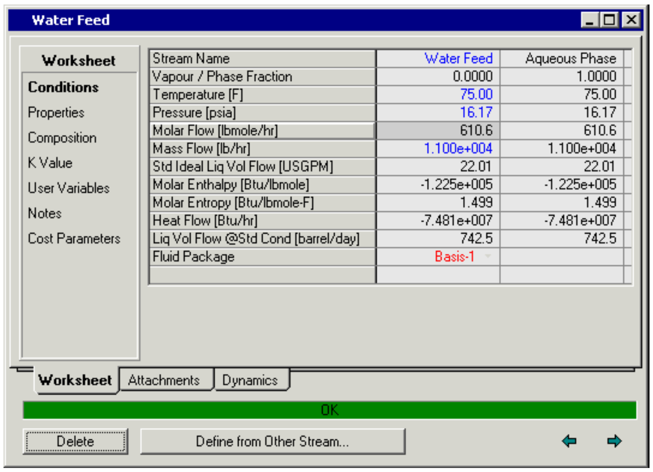
10. Click the **Conditions** page to view the calculated stream properties. You can display the properties of all phases by resizing the property view



Sizing Arrow Icon

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

Figure 3.46



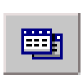
New or updated information is automatically and instantly transferred among all locations in UniSim Design.

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

13. 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.



Workbook Icon

Installing the Mixer

The first operation is a **Mixer**, used to combine the two feed streams. As with most commands in UniSim Design, installing an operation can be accomplished in a number of ways. One method is through the Unit Ops tab of the Workbook.

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.

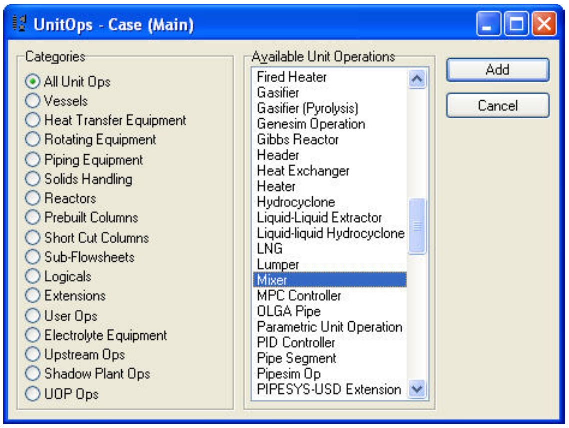
To add an operation, you can double-clicking on a listed operation.

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, UniSim Design 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.

Figure 3.47

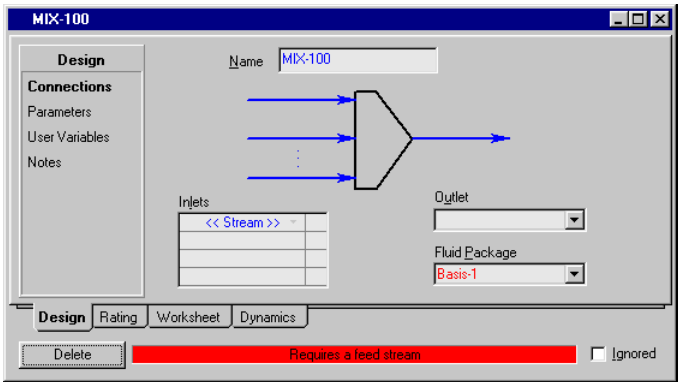


5. With Mixer selected, click the **Add** button, or press **ENTER**.

   The property view for the **Mixer** appears.

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

Figure 3.48



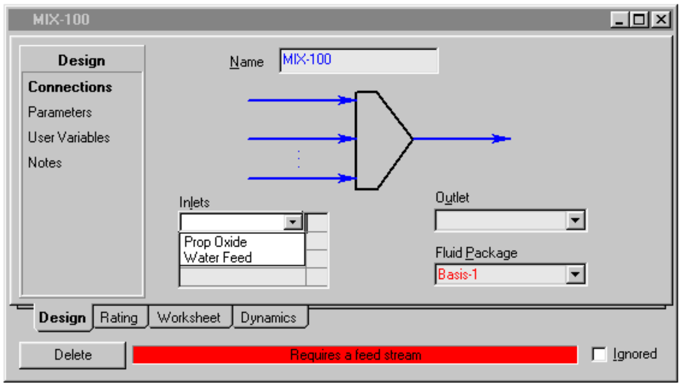
The unit operation property view contains all the information required to define the operation, organized into tabs and pages. The **Design**, **Rating**, **Worksheet,** and **Dynamics tabs** appear in the property view for most operations. Property views for more complex operations contain more tabs. UniSim Design 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 the **DOWN** arrow key.

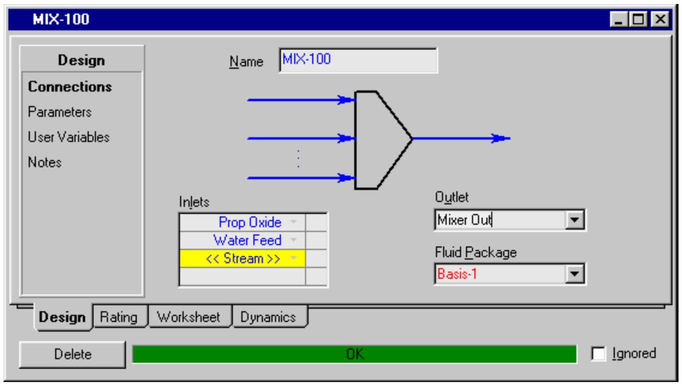
Figure 3.49



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**. UniSim Design recognizes that there is no existing stream with this name, so it creates the new stream.

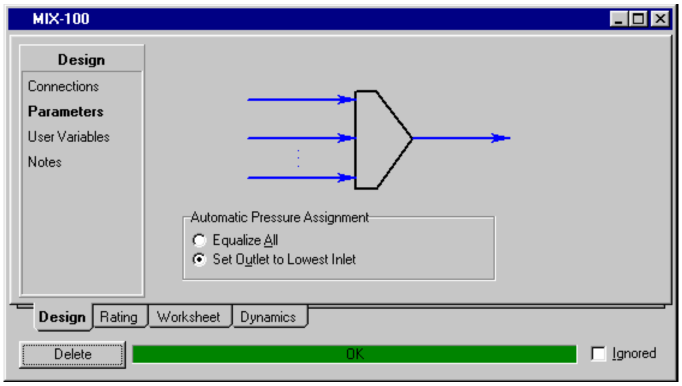
Figure 3.50



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**.

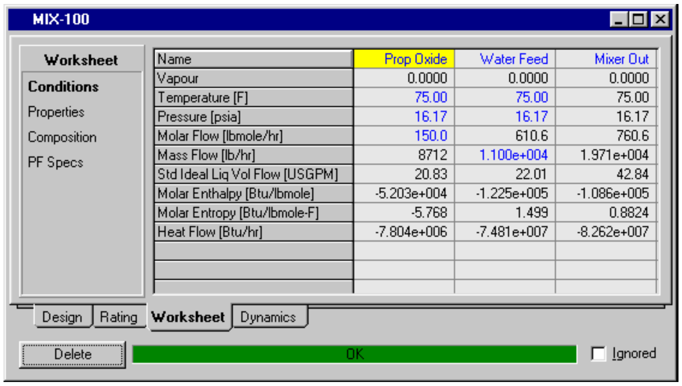
Figure 3.51



UniSim Design 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.

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.

Figure 3.52

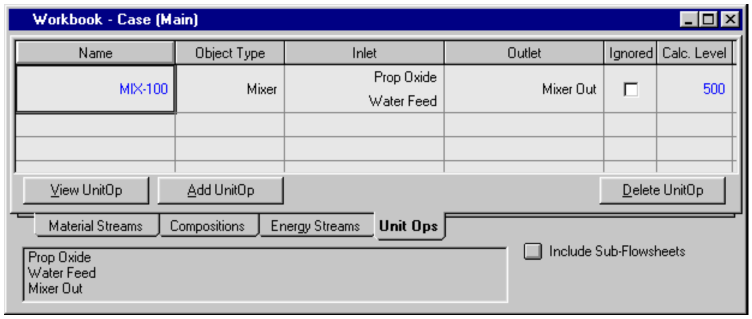


Name	Prop Oxide	Water Feed	Mixer Out
Vapour	0.0000	0.0000	0.0000
Temperature [F]	75.00	75.00	75.00
Pressure [psia]	16.17	16.17	16.17
Molar Flow [lbmole/hr]	150.0	610.6	760.6
Mass Flow [lb/hr]	8712	1.100e+004	1.971e+004
Std Ideal Liq Vol Flow [USGPM]	20.83	22.01	42.84
Molar Enthalpy [Btu/lbmole]	-5.203e+004	-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 and UnitOps view to return to the Workbook.

16. The new operation appears in the table of the Workbook **Unit Ops** tab.

Figure 3.53



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, 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 the 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.

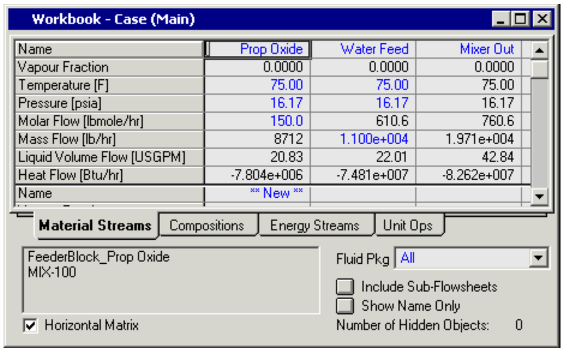
Any utilities attached to the stream with focus in the **Workbook** are also displayed in (and are accessible from) this box.

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.

1. To access the property view for the Mixer, double-click on its name in the gray box.

Figure 3.54



Adding a Tab to the Workbook

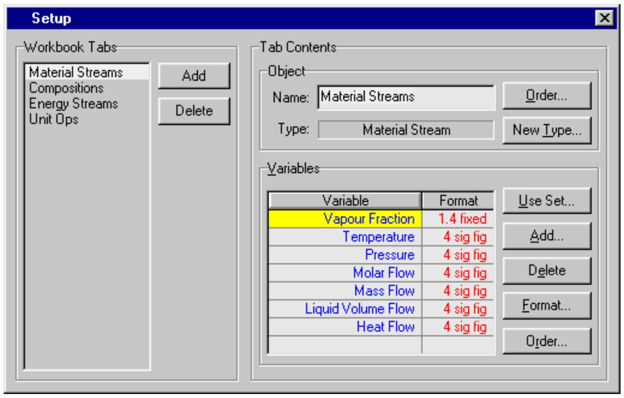
When the **Workbook is active**, the **Workbook** item appears in the UniSim Design menu bar. This item allows you to customize the **Workbook**.

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.

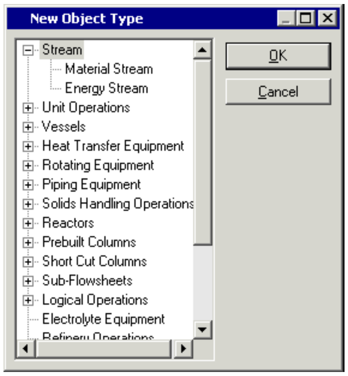
Figure 3.55



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.

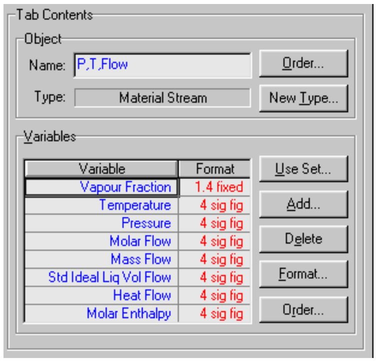
Figure 3.56



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 3.57

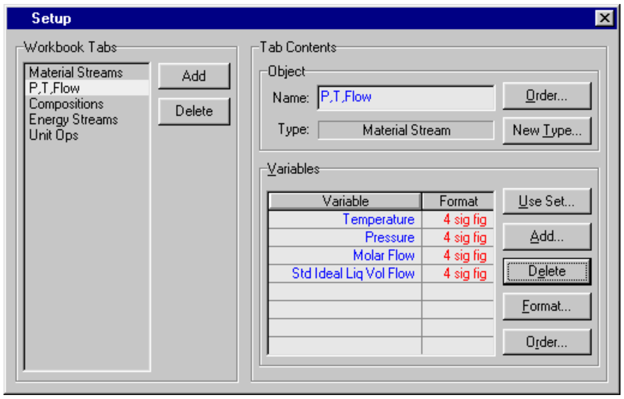


The next task is to customize the tab by removing the variables that are irrelevant.

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.

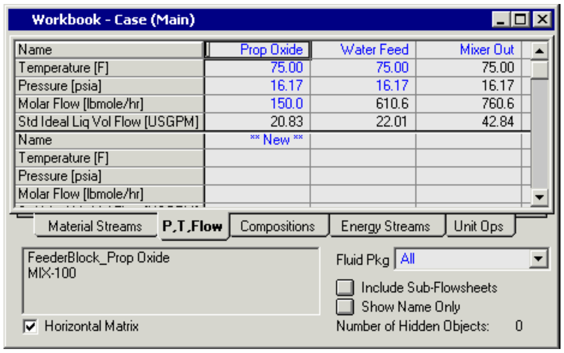
If you want to remove variables from another tab, you must edit each tab individually.

Figure 3.58



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

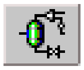
Figure 3.59



12. Save the case.

3.2.7 Installing Equipment on the PFD

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

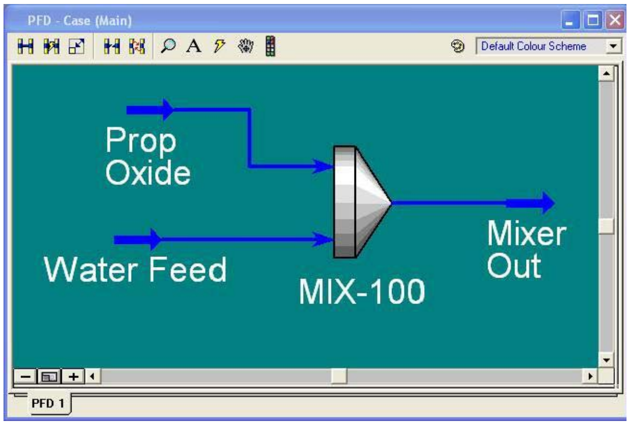


PFD Icon

1. To open the PFD, click the **PFD** icon on the toolbar. The PFD item appears in the UniSim Design menu bar whenever the PFD has focus.

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

Figure 3.60

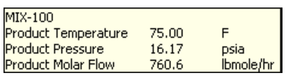


Like any other non-modal view, the PFD view can be re-sized by clicking and dragging anywhere on the outside border.

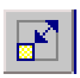
As a graphical representation of your flowsheet, the PFD shows the connections among all streams and operations, also known as

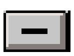
"objects". Each object is represented by a symbol, also known as an "icon". A stream icon is an arrow pointing in the direction of flow, while an operation icon is a graphic representing the actual physical operation. The object name, also known as a "label", appears near each icon.

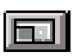
The PFD shown above has been rearranged by moving the **Prop Oxide** feed stream icon up slightly so it does not overlap the **Water Feed stream** icon. To move an icon, simply click and drag it to a new location. You can click and drag either the icon (arrow) itself, or the label (object name), as these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

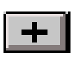


Fly-by information


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 **UniSim Design User Guide**.

Calculation Status

UniSim Design 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 UniSim Design 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.

Indicator Status	Description
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.

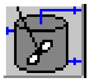
Notice that the icons for all streams installed to this point are dark blue.

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.

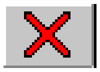
Installing the Reactor

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.



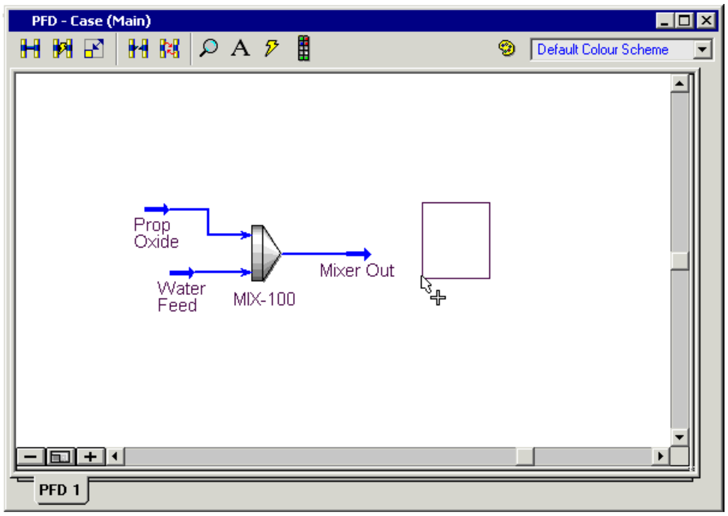
CSTR Icon



Cancel Icon

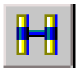
4. Position the cursor in the **PFD** to the right of the **Mixer Out** stream. The cursor changes to a special cursor with a plus (+) symbol attached to it. The symbol indicates the location of the operation icon.

Figure 3.61



5. Click to “drop” the **Reactor** onto the **PFD**. UniSim Design 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

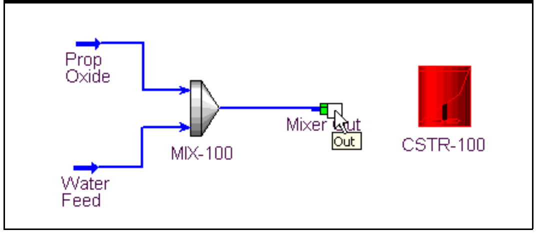
1. Click the **Attach Mode** icon on the **PFD** toolbar to enter **Attach** mode.

   The Attach Mode button stays active until you click it again to return to **Move** mode.

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

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 3.62

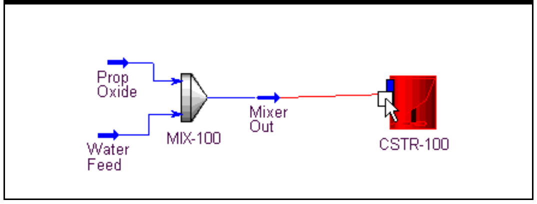


3. With the pop-up ‘Out’ visible, click and hold the mouse button. The transparent box becomes solid black, indicating that you are beginning a connection.

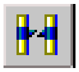
Multiple connection points appear because the Reactor accepts multiple feed streams.

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 3.63



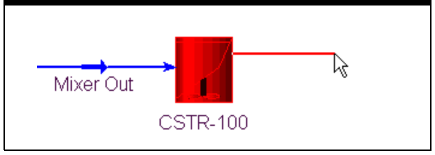
6. Release the mouse button, and the connection is made between the stream and the **CSTR-100** inlet.
7. Position the cursor over top right-hand corner of the **CSTR-100** icon. The white box and the pop-up ‘Vapour Product’ appear.
8. With the pop-up visible, left-click and hold. The white box again 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 3.64



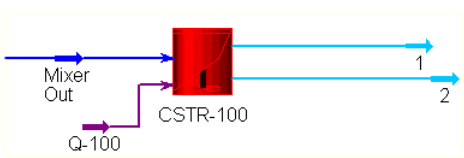
10. With the stream icon visible, release the left mouse button. UniSim Design creates a new stream with the default name **1**.
11. Place the cursor over the bottom right connection point on the reactor labeled 'Liquid Product', then click and drag to the right to create the reactor's liquid product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

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

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.

Figure 3.65



13. Click the **Attach Mode** icon again to return to **Move** mode.
14. Double-click the stream 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.

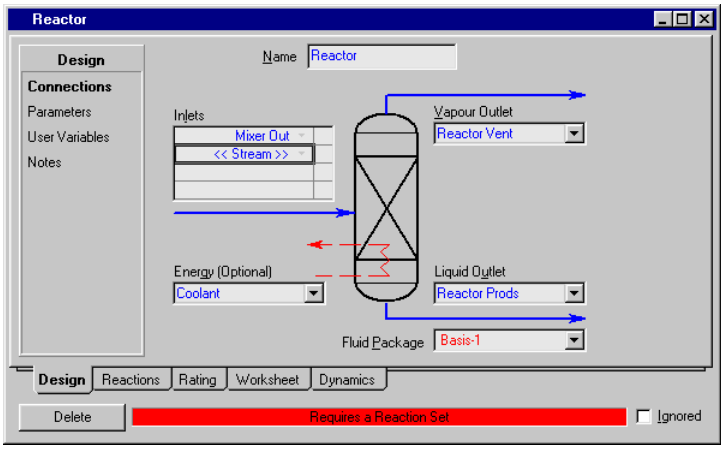
    The reactor outlet and energy streams are unknown at this point, so they are light blue and purple, respectively.

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.

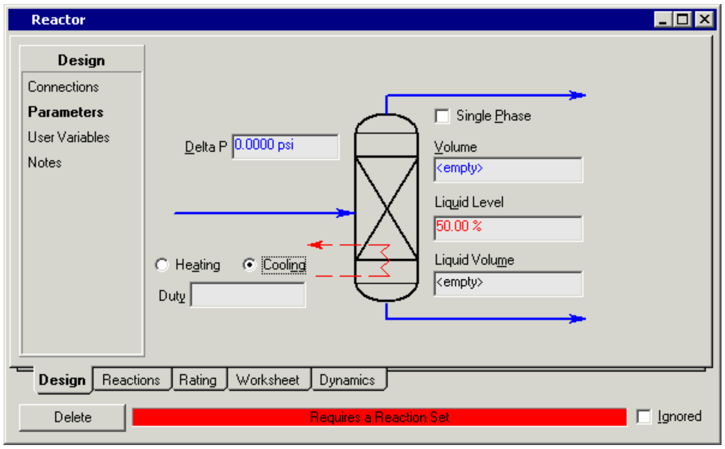
3. In the **Name** cell, change the operation **name** to **Reactor**.

Figure 3.66



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.

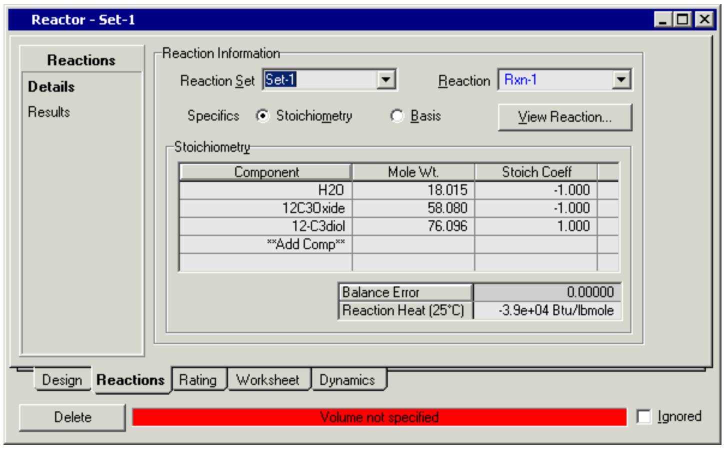
Figure 3.67



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 3.68

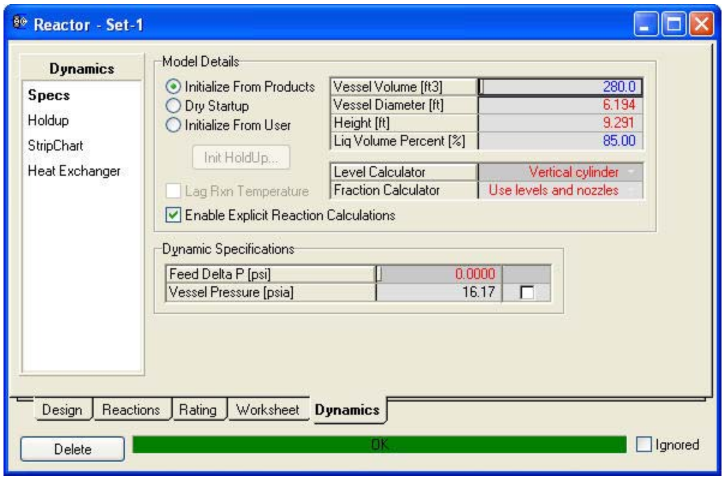


The next task is to specify the **Vessel Parameters**. In this Tutorial, the reactor has a volume of 280 ft3 and is 85% full.

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**.

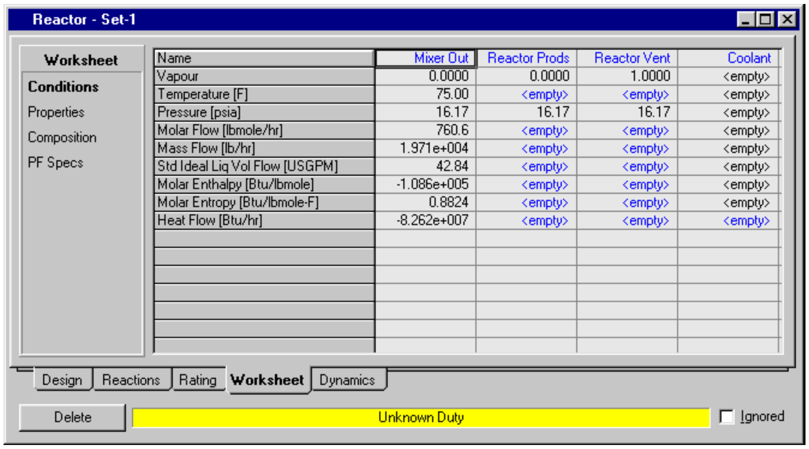
UniSim Design automatically calculates the **Liquid Volume** in the vessel (280 ft3 x 85% full = 238 ft3), displayed on the **Parameters** page of the **Design** tab.

Figure 3.69



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

Figure 3.70

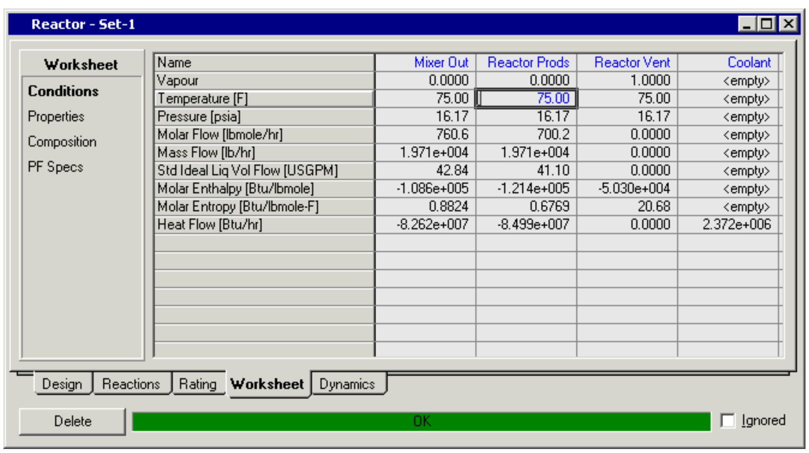


At this point, the **Reactor** product streams and the energy stream **Coolant** are unknown because the **Reactor** has one degree of freedom. At this point, either the outlet stream temperature or the cooling duty can be specified. For this example, you will specify the outlet temperature.

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**. UniSim Design solves the Reactor.

Figure 3.71

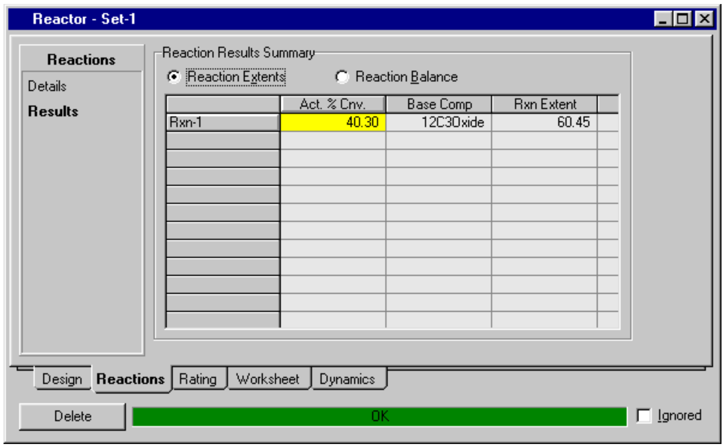


There is no phase change in the Reactor under isothermal conditions since the flow of the vapour product stream **Reactor**

Vent is zero. In addition, the required cooling duty has been calculated and is represented by the Heat Flow of the **Coolant** stream. 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.

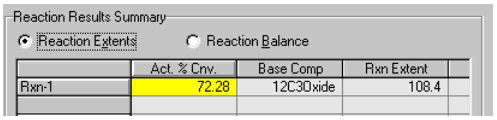
Figure 3.72



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.

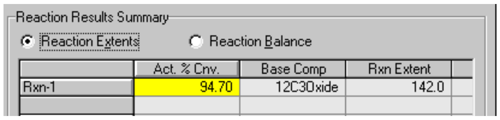
Figure 3.73



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.

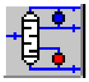
Figure 3.74



19. Close the **Reactor** property view.

Installing the Column

UniSim Design 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.



Distillation Column Icon

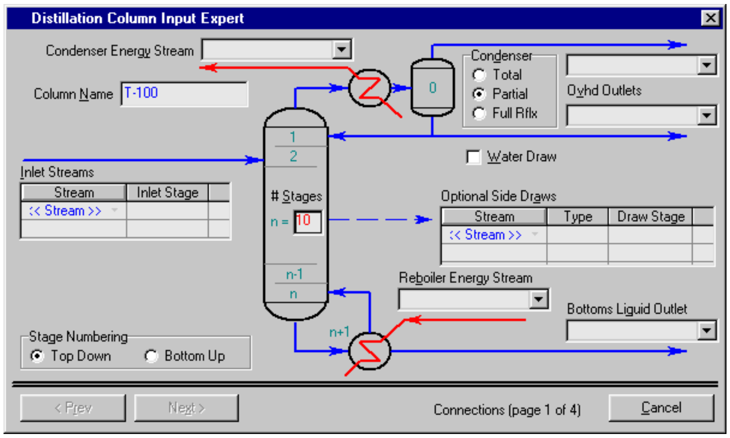
1. Before installing the column, click the **Tools** menu and select **Preferences**.
2. On the **Simulation** tab, click on the **Options** page and ensure that the **Use Input Experts** checkbox is selected (checked), then close the view.
3. Double-click the **Distillation Column** icon on the **Object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

   The first page of the **Input Expert** appears.

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 3.75



4. For this example, 10 theoretical stages are used, so leave the **# Stages** at its default value.
5. In the Inlet Streams table, click in the **<<Stream>>** cell.

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

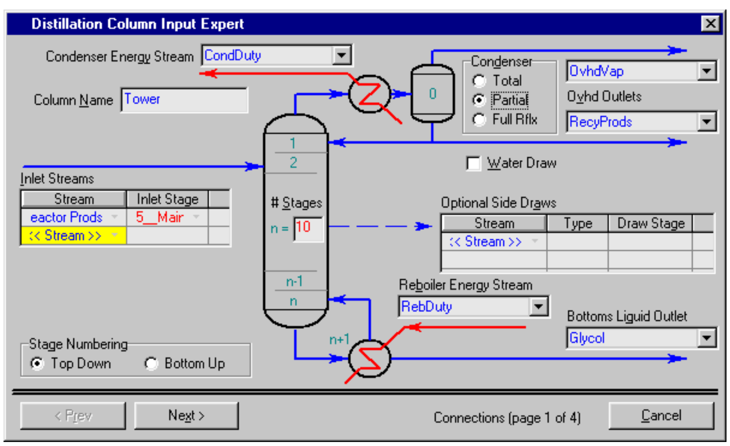
- These are theoretical stages, as the UniSim Design default stage efficiency is one.
- The Condenser and Reboiler are considered separate from the other stages, and are not included in the **# Stages**.

6. From the drop-down list of available inlet streams, select **Reactor Prods** as the feed stream to the column. UniSim Design supplies a default feed location in the middle of the Tray Section (TS), in this case stage 5 (indicated by **5_Main TS**).
7. In the **Condenser** group, ensure the **Partial** radio button is selected, as the column will have both Vapour and Liquid Overhead Outlets.
8. In the **Column Name** field, change the name to **Tower**.
9. In the **Condenser Energy Stream** field, type CondDuty, then press **ENTER**.
10. In the top **Ovhd Outlets** field, type OvhdVap, then press **ENTER**.

    In the bottom **Ovhd Outlets** field, type RecyProds, then press **ENTER**.
11. In the **Reboiler Energy Stream** field, type RebDuty, then press **ENTER**.
12. 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.**

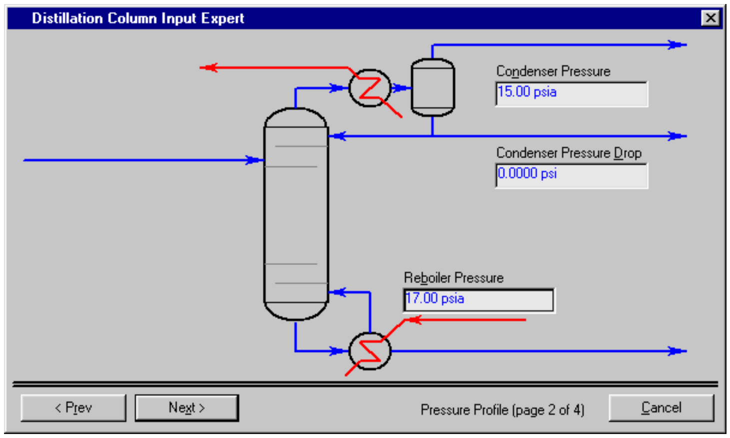
Figure 3.76



13. Click the **Next** button to advance to the **Pressure Profile** page.
14. In the **Condenser Pressure** field, enter 15 psia.
15. In the **Reboiler Pressure** field, enter 17 psia.

Leave the **Condenser Pressure Drop** at its default value of zero.

Figure 3.77



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

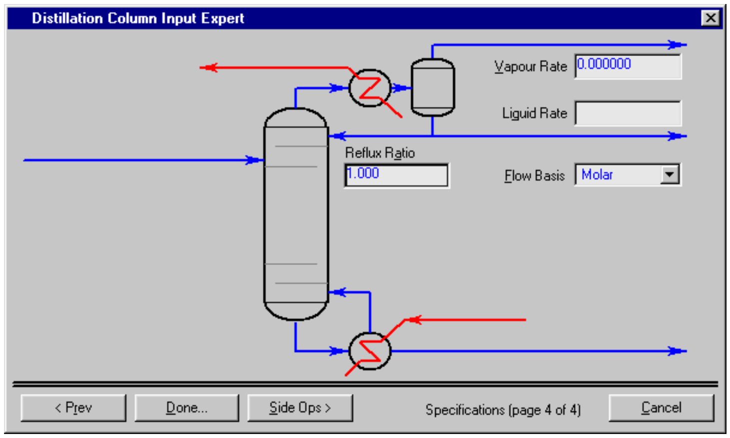
16. Click the **Next** button to advance to the **Optional Estimates** page. For this example, no estimates are required.
17. Click the **Next** button to advance to the fourth and final page of the Input Expert. This page allows you to supply values for the default column specifications that UniSim Design 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.**

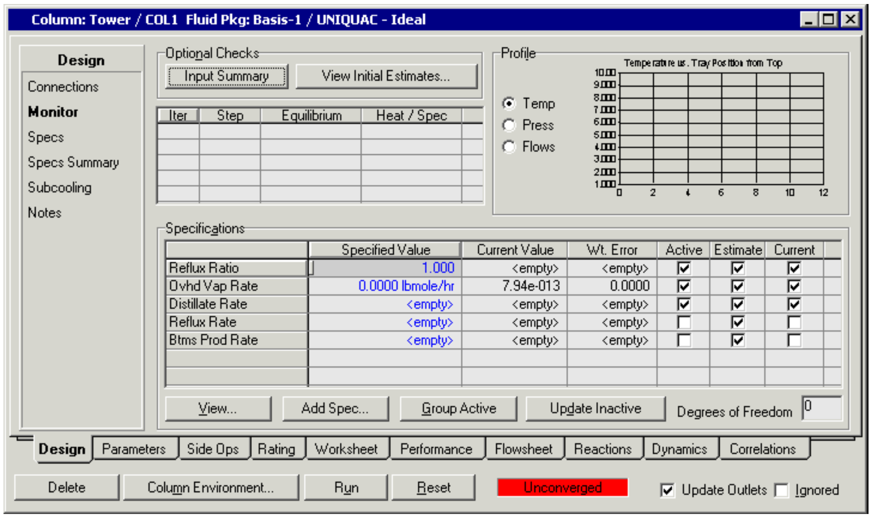
18. In the **Vapour Rate** field, enter **0** lbmole/hr.
19. **In the Reflux Ratio** field, enter **1.0**.

Figure 3.78



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

Figure 3.79



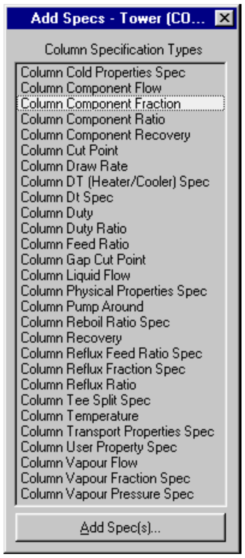
You can also change specification values, and activate or de-activate specifications used by the Column solver directly from the **Monitor** page.

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

Adding a Column Specification

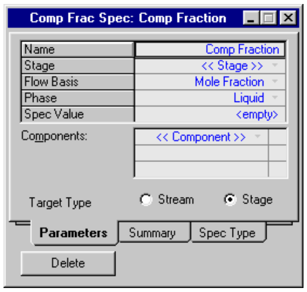
The current Degrees of Freedom is zero, indicating the column is ready to be run, however, the Distillate Rate (Overhead Liquid Rate for which no value was provided in the Input Expert) is currently an Active specification with a Specified Value of <empty>. For this example, you will specify a water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



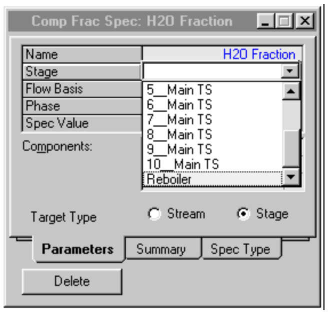
5. Click the **Add Spec(s)** button. The Comp Frac Spec view appears.

Figure 3.80



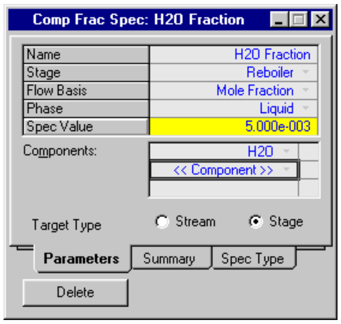
6. In the **Name** cell, change the name to **H2O Fraction**.
7. In the **Stage** cell, select **Reboiler** from the drop-down list.

Figure 3.81



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 3.82



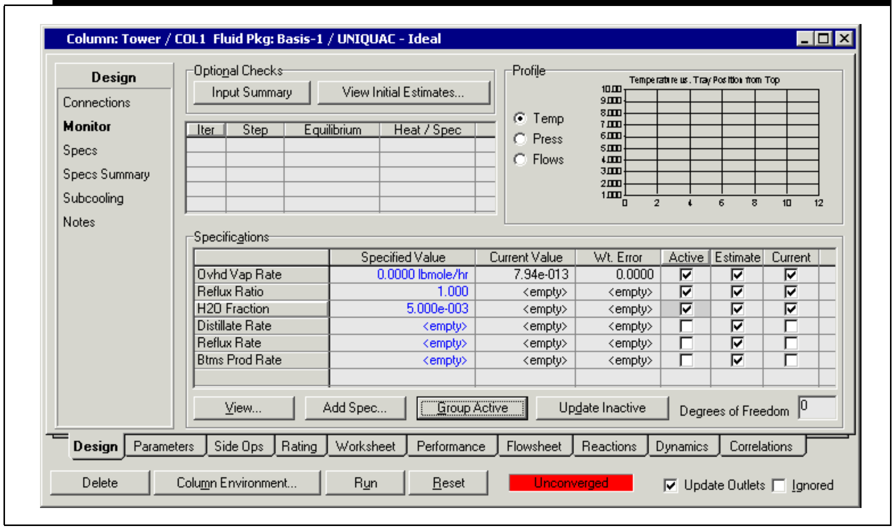
10. Close this view to return to the Column property view. The new specification appears in the **Column Specifications** list on the **Specs** page.

11. Return to the **Monitor** page, where the new specification appears at the bottom of the Specifications list.

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

12. Click the **Group Active** button to bring the new specification to the top of the list, directly under the other Active specifications.

Figure 3.83



UniSim Design automatically made the new specification **Active** when you created it.

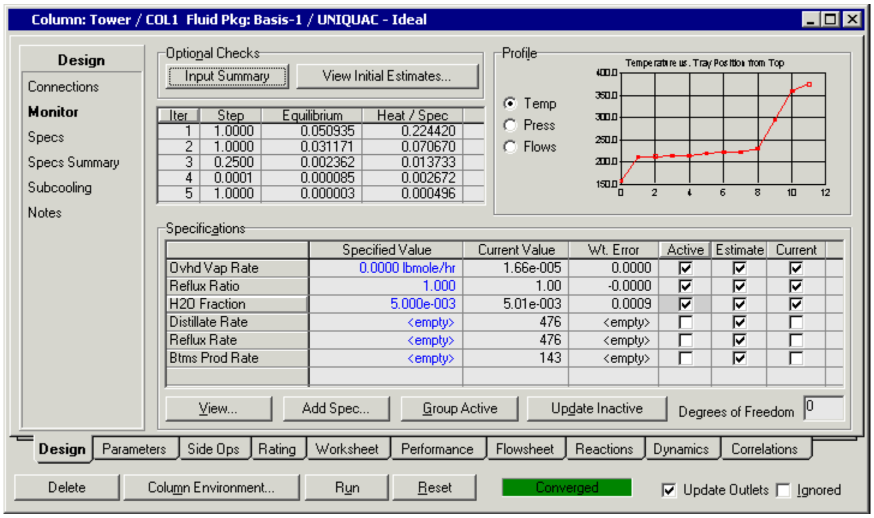
The **Degrees of Freedom** has returned to zero, so the column is ready to be calculated.

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.

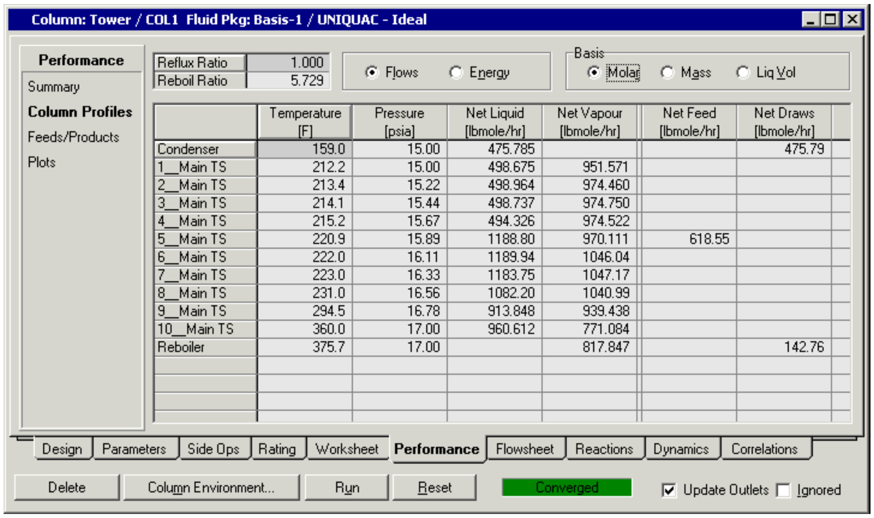
Figure 3.84



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

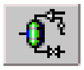
2. Select the **Press** or **Flows** radio button to view the pressure or flow profiles.
3. To access a more detailed stage summary, click the **Performance** tab, then select the **Column Profiles** page.

Figure 3.85

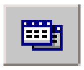


Accessing the Column Sub-flowsheet

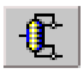
When considering the column, you might want to focus only on the column sub-flowsheet. You can do this by entering the column environment.



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 3.86

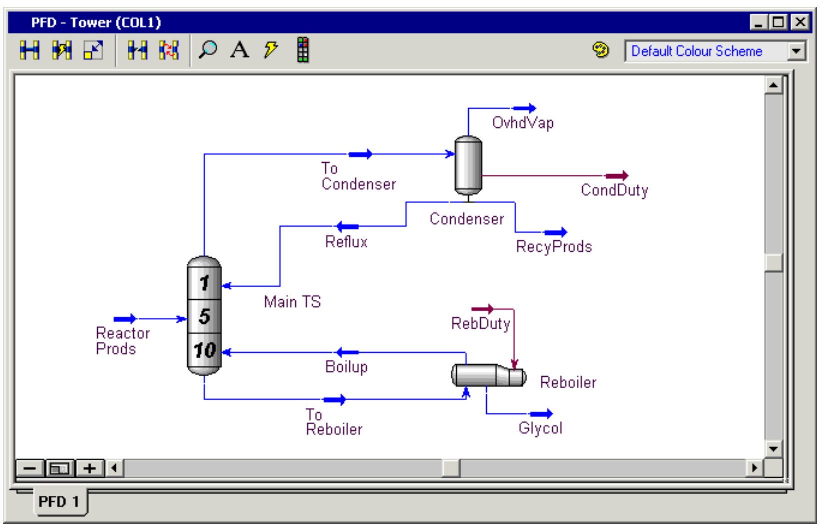
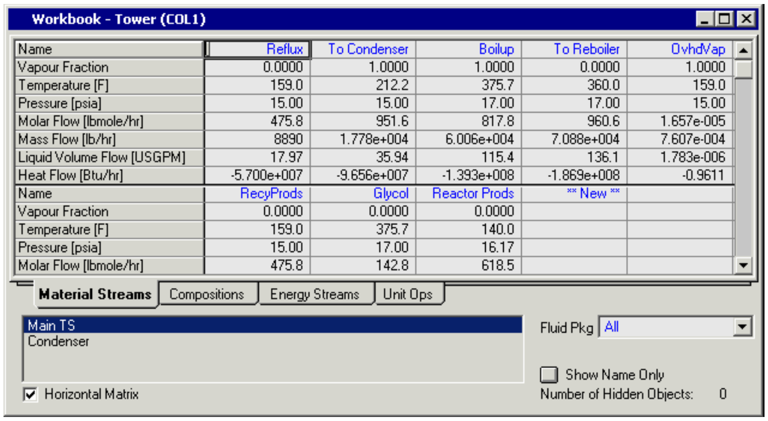
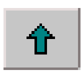


Figure 3.87



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	1.657e-005
Mass Flow [lb/hr]	8890	1.778e+004	6.006e+004	7.088e+004	7.607e-004
Liquid Volume Flow [USGPM]	17.97	35.94	115.4	136.1	1.783e-006
Heat Flow [Btu/hr]	-5.700e+007	-9.656e+007	-1.393e+008	-1.869e+008	-0.9611
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		



Enter Parent Simulation Environment Icon

2. When you are finished in the column environment, return to the Main Flowsheet by clicking the **Enter Parent Simulation Environment** icon.
3. Open the **PFD** for the Main Flowsheet and select **Auto Position All** from the **PFD** menu. UniSim Design arranges your **PFD** in a logical manner.

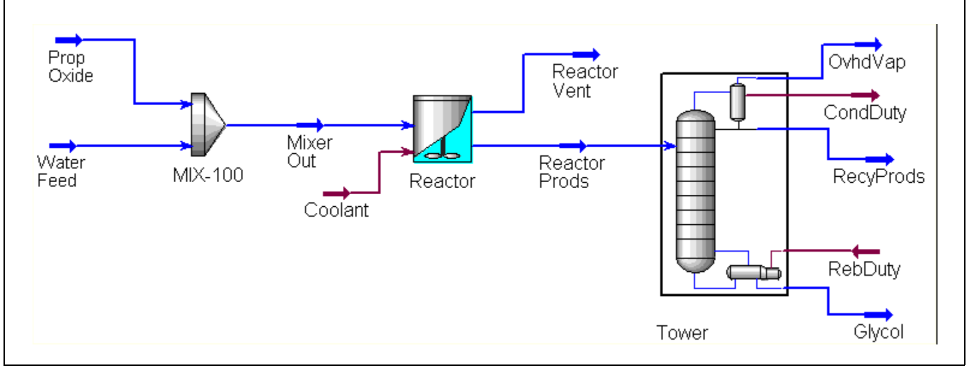
Moving Objects and Labels in a PFD

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 3.88

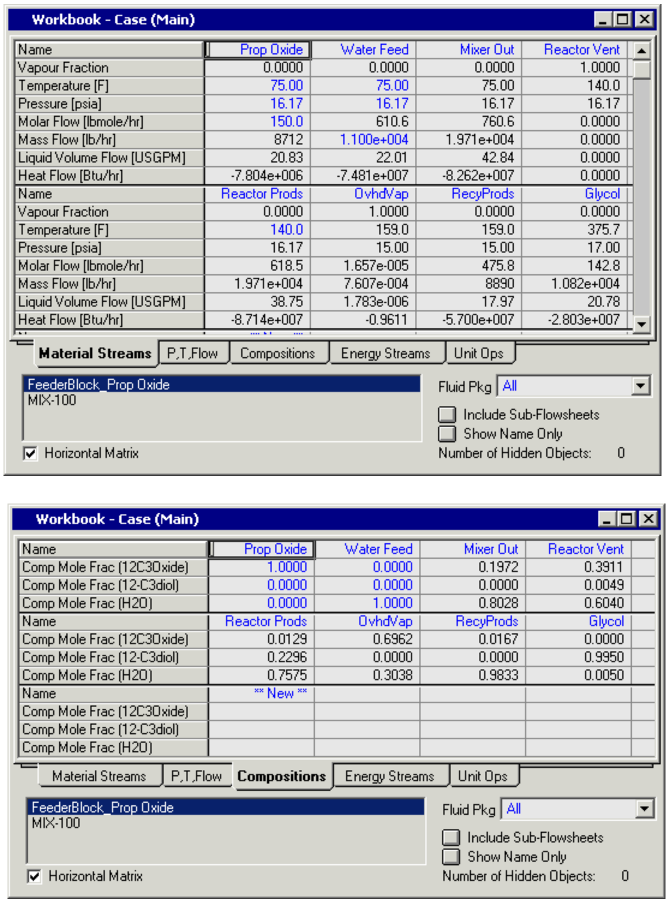


3.2.8 Viewing Results

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 3.89

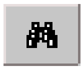


Name	Prop Oxide	Water Feed	Mixer Out	Reactor Vent
Vapour Fraction	0.0000	0.0000	0.0000	1.0000
Temperature [F]	75.00	75.00	75.00	140.0
Pressure [psia]	16.17	16.17	16.17	16.17
Molar Flow [lbmole/hr]	150.0	610.6	760.6	0.0000
Mass Flow [lb/hr]	8712	1.100e+004	1.971e+004	0.0000
Liquid Volume Flow [USGPM]	20.83	22.01	42.84	0.0000
Heat Flow [Btu/hr]	-7.804e+006	-7.481e+007	-8.262e+007	0.0000
Name	Reactor Prods	OvhdVap	RecyProds	Glycol
Vapour Fraction	0.0000	1.0000	0.0000	0.0000
Temperature [F]	140.0	159.0	159.0	375.7
Pressure [psia]	16.17	15.00	15.00	17.00
Molar Flow [lbmole/hr]	618.5	1.657e-005	475.8	142.8
Mass Flow [lb/hr]	1.971e+004	7.607e-004	8890	1.082e+004
Liquid Volume Flow [USGPM]	38.75	1.783e-006	17.97	20.78
Heat Flow [Btu/hr]	-8.714e+007	-0.9611	-5.700e+007	-2.803e+007

Name	Prop Oxide	Water Feed	Mixer Out	Reactor Vent
Comp Mole Frac (12C3Oxide)	1.0000	0.0000	0.1972	0.3911
Comp Mole Frac (12-C3diol)	0.0000	0.0000	0.0000	0.0049
Comp Mole Frac (H2O)	0.0000	1.0000	0.8028	0.6040
Name	Reactor Prods	OvhdVap	RecyProds	Glycol
Comp Mole Frac (12C3Oxide)	0.0129	0.6962	0.0167	0.0000
Comp Mole Frac (12-C3diol)	0.2296	0.0000	0.0000	0.9950
Comp Mole Frac (H2O)	0.7575	0.3038	0.9833	0.0050
Name	** New **			
Comp Mole Frac (12C3Oxide)				
Comp Mole Frac (12-C3diol)				
Comp Mole Frac (H2O)				

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.



Object Navigator Icon

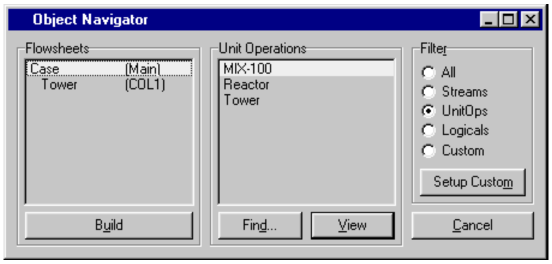
1. To open the Navigator, do **one** of the following:
   - Click the **Object Navigator** icon.
   - Press **F3**.

- From the Flowsheet menu, select **Find Object**.
- Double-click on any blank space on the UniSim Design Desktop.

The **Object Navigator** view appears.

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.

Figure 3.90



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

2. To open a property view, select the operation in the list, then click the View button or double-click on the operation name.
3. You can also search for an object by clicking the Find button.
4. When the Find Object view appears, enter the object name, then click the OK button. UniSim Design opens the property view for the object you specified

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.

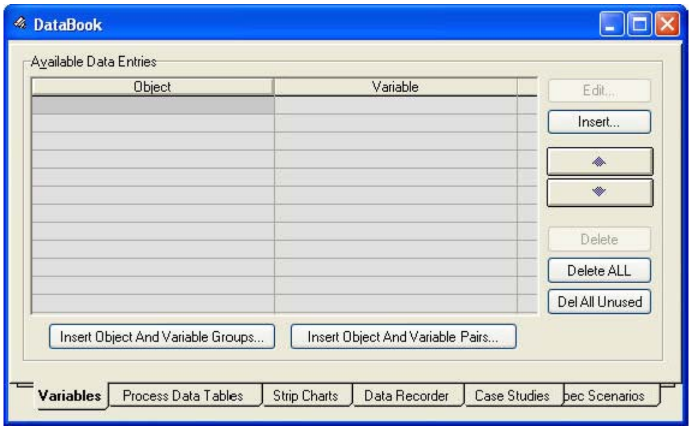
Using the Databook

The UniSim Design 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 3.91



To edit any of the Objects in the Databook:

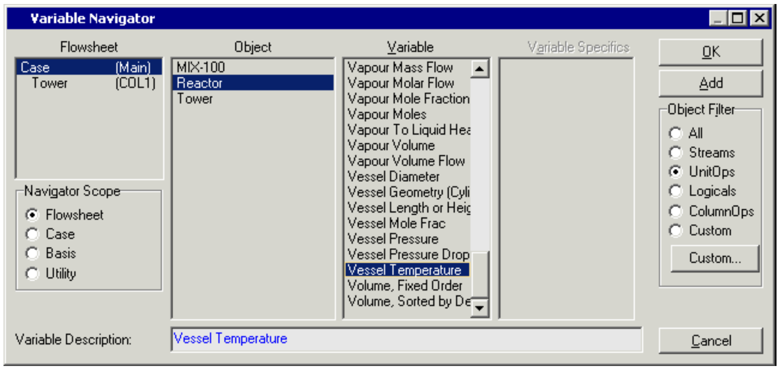
1. Select the Object you want to edit.
2. Click the **Edit** button.

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

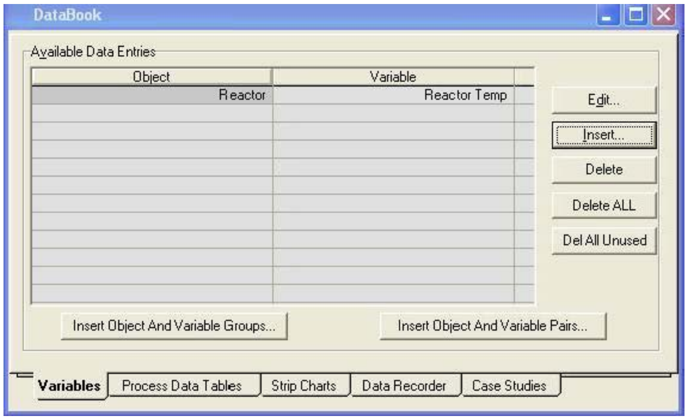
The Variable Navigator is used extensively in UniSim Design for locating and selecting variables. The Navigator operates in a left-to-right manner—the selected Flowsheet determines the Object list, the chosen Object dictates the Variable list, and the selected Variable determines whether any Variable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

Figure 3.92



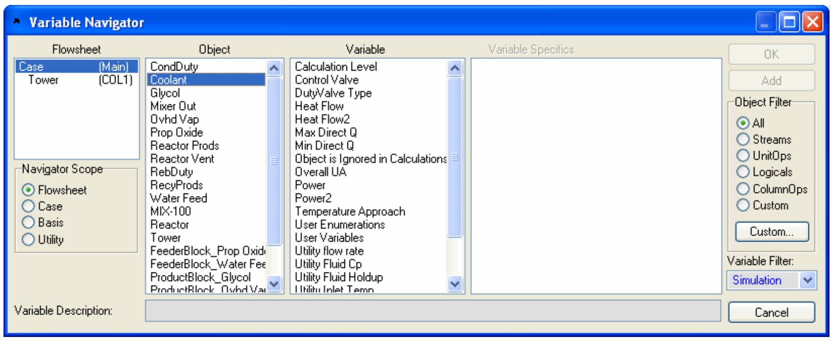
7. In the **Variable Description** field, rename the variable **Reactor Temp**, then click the **OK** button. The variable now appears in the **Databook**.

Figure 3.93



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.

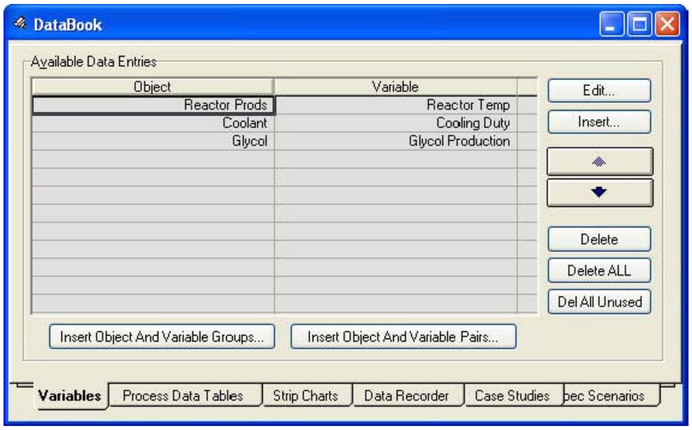
Figure 3.94



12. In the **Variable Description** field, change the description to **Cooling Duty**, then click the **Add** button. The variable now appears in the **Databook** and the Variable Navigator view remains open.
13. 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 **Add** button.

14. Click the **Close** button to return to the Databook view. The completed **Variables** tab of the **Databook** appears below.

Figure 3.95



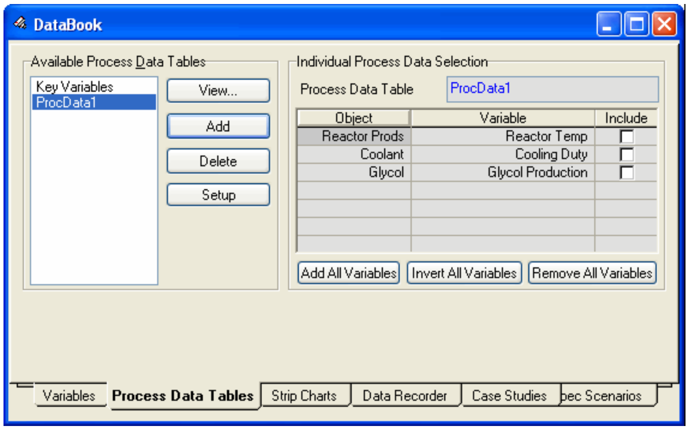
Now that the key variables have been added to the **Databook**, the next task is to create a data table in which to display these variables.

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

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

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

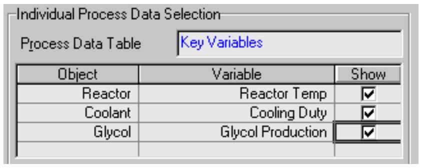
Figure 3.96



17. In the **Process Data Table** field, change the name to **Key Variables**.

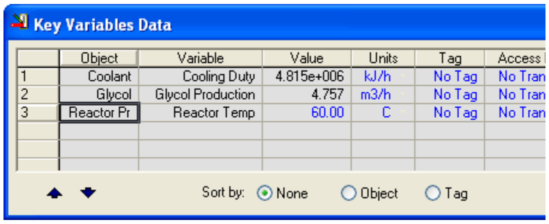
18. In the Show column, activate each variable by clicking on the corresponding checkbox.

Figure 3.97



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

Figure 3.98



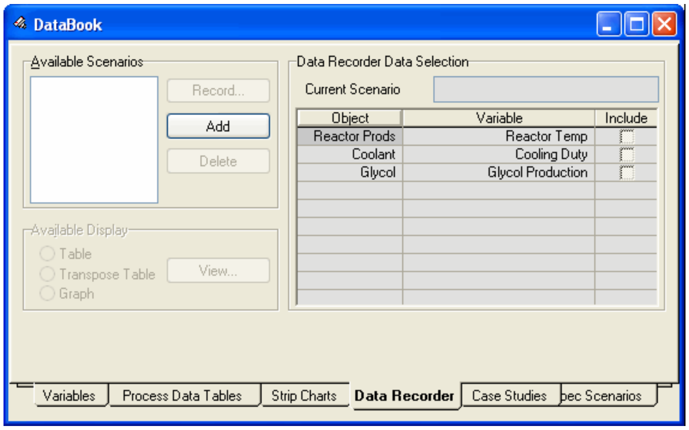
This table will be accessed again later to demonstrate how its results are updated whenever a flowsheet change is made.

20. For now, click the **Minimize** icon in the upper right corner of the **Key Variables Data** view. UniSim Design 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.

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

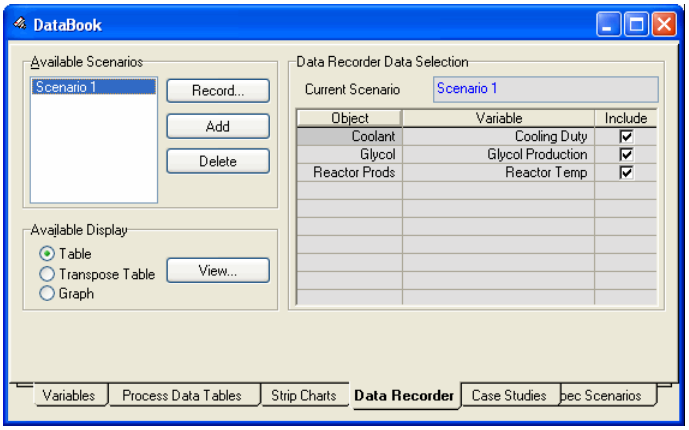
Figure 3.99



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.

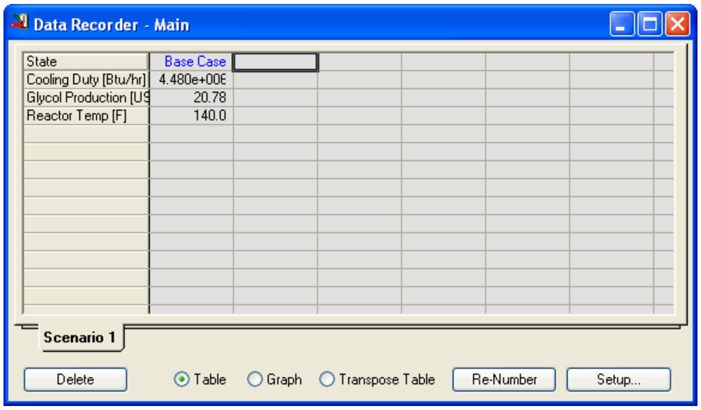
22. In the **Available Scenarios** group, click the **Add** button. UniSim Design creates a new scenario with the default name Scenario 1.
23. In the Data Recorder Data Section group, activate each variable by clicking on the corresponding **Include** checkbox.

Figure 3.100



24. 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.
25. In the **Name for New State** field, change the name **to Base Case**, then click **OK**. You return to the **Databook**.
26. 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.

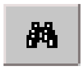
Figure 3.101



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.

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

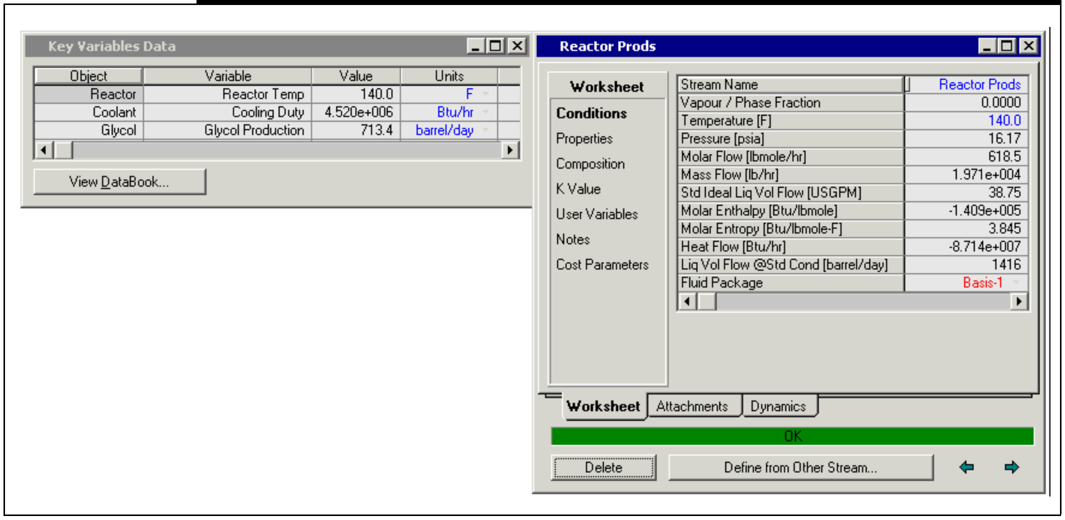
Next, you will change the temperature of stream **Reactor Prods** (which determines the **Reactor** temperature), then view the changes in the process data table



Object Navigator Icon

29. Click the **Object Navigator** icon in the toolbar.
30. In the Filter group, select the **Streams** radio button.
31. In the Streams list, select **Reactor Prods**, then click the **View** button. The **Reactor Prods** property view appears.
32. Ensure you are on the **Worksheet** tab, **Conditions** page of the property view.
33. Arrange the Reactor Prods and Key Variables Data views so you can see them both.

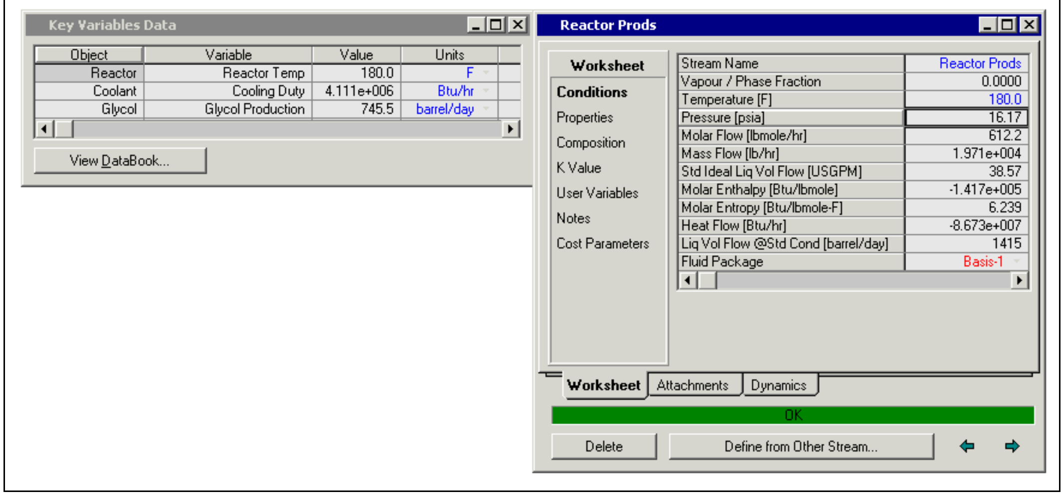
Figure 3.102



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

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

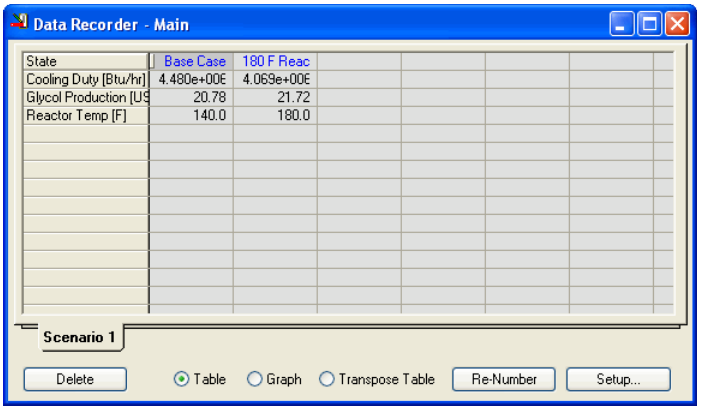
Figure 3.103



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

35. 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.
36. Click on the **Data Recorder** tab in the **Databook**.
37. Click the **Record** button. The New Solved State view appears.
38. In the **Name for New State** field, change the name to **180F Reactor**, then click the **OK** button.
39. In the Available Display group, click the **View** button. The **Data Recorder** appears, displaying the new values of the variables.

Figure 3.104



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

    This completes the UniSim Design 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 UniSim Design.

3.3 Dynamic Simulation

A completed dynamic case has been pre-built and is located in the file **dynTUT3.usc** in your UniSim Design\Samples directory.

In this tutorial, the dynamic capabilities of UniSim Design will be incorporated into a basic steady state chemicals model. In the steady state simulation, a continuously-stirred tank reactor (CSTR) converted propylene oxide and water into propylene glycol. The reactor products were then fed into a distillation tower where the glycol product was recovered in the tower bottoms.

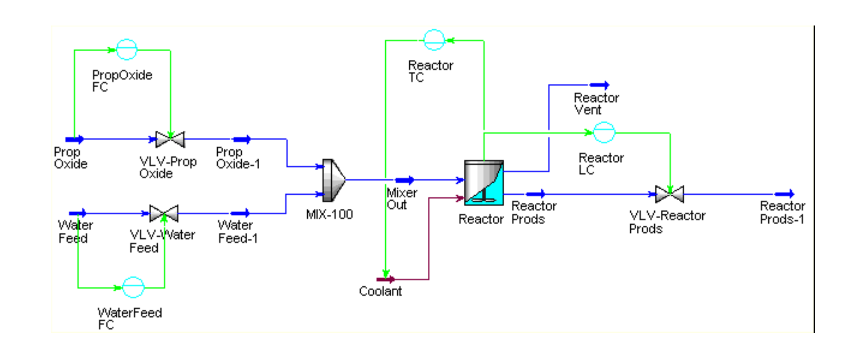
This tutorial follows these basic steps for setting up a dynamic simulation case:

1. Obtain a simplified steady state model to be converted to dynamic mode.
2. Use the Dynamic Assistant to set pressure-flow specifications, modify the flowsheet topology, and size the equipment.
3. Modify the Reactor vent stream to account for reverse flow conditions.
4. Set up temperature and level controllers around and in the Reactor vessel.
5. Set up the Databook. Make changes to key variables in the process and observe the dynamic behaviour of the model.

The dynamic simulation will take the steady state CSTR simulation case and convert it into dynamic mode. If you have not built the simulation for the steady state simulation, you can open the pre-built case included with your UniSim Design package.

A flowsheet of the completed dynamic simulation is shown in the figure below.

Figure 3.105



Only the CSTR reactor will be converted to dynamic mode. The Column operation will be deleted from the simulation flowsheet.

The Dynamics Assistant will be used to make pressure-flow specifications, modify the flowsheet topology, and size pieces of equipment in the simulation flowsheet. This is only **one** method of preparing a steady state case for dynamic mode. It is also possible to set your own pressure-flow specifications and size the equipment without the aid of the Dynamic Assistant.

3.3.1 Simplifying the Steady State Flowsheet

The distillation column in the Chemicals Tutorial will be deleted in this section.

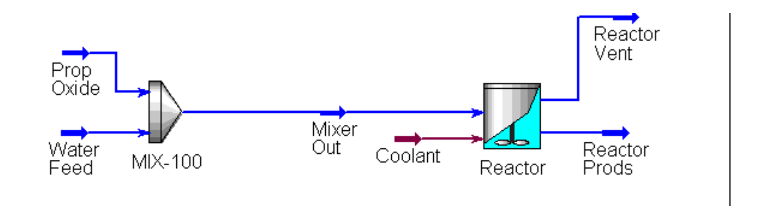
1. Open the pre-built case file **TUTOR3.usc** located in your UniSim Design\Samples directory (if you are not continuing from the Steady State Simulation section of this tutorial).
2. From the **Tools** menu, select **Preferences**.
3. Click the **Variables** tab, then select the **Units** page.
4. In the Available Unit Sets group, select Field. Close the Session Preferences view.
5. From the **File** menu, select **Save As**.
   Save the case as **DynTUT3-1.usc**.
6. Delete all material streams and unit operations downstream of the Reactor Prods stream. The following 6 items should be deleted:

When you delete a stream, unit or logical operation from the flowsheet, UniSim Design will ask you to confirm the deletion. To delete the object, click the **Yes** button. If not, click the **No** button.

Material Streams	Energy Streams	Unit Operations
Ovhd Vap **RecyProds** **Glycol**	CondDuty RebDuty	Tower

7. The steady state simulation case should solve with the deletion of the above items. The PFD for the dynamic tutorial should appear as shown below.

Figure 3.106



Before entering dynamics, the pressure specification on the Water Feed stream should be removed so that the MIX-100 unit operation can calculate its pressure based on the Prop Oxide stream

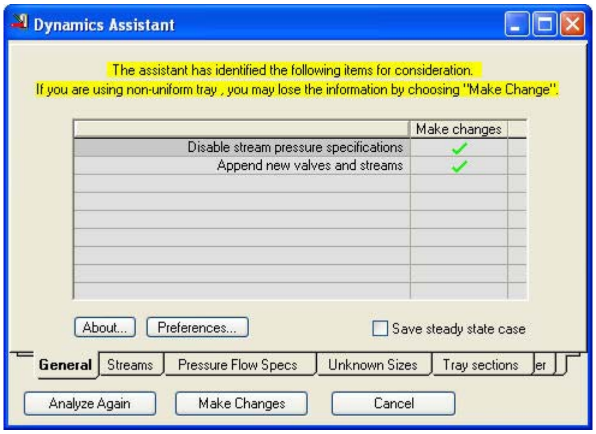
specification.

8. Double-click the Water Feed stream icon to open its property view.
9. On the **Conditions** page of the **Worksheet** tab, click in the **Pressure** cell, then press **DELETE**.
10. Close the Water Feed stream property view.
11. Double-click the MIX-100 icon to open its property view.
12. Click the **Design** tab, then select the **Parameters** page.
13. In the Automatic Pressure Assignment group, select the **Equalize All** radio button. UniSim Design solves for the stream and mixer operation.
14. Close the mixer property view.
15. Save the case.

3.3.2 Using the Dynamics Assistant

The Dynamics Assistant makes recommendations as to how the flowsheet topology should change and what pressure-flow specifications are required in order to run a case in dynamic mode. In addition, it automatically sets the sizing parameters of the equipment in the simulation flowsheet. Not all the suggestions the Dynamics Assistant offers need to be followed.

Figure 3.107



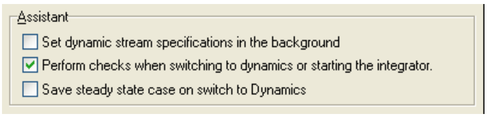
The Dynamics Assistant will be used to do the following:

- Add Pressure Flow specifications to the simulation case.
- Add Valves to the Boundary Feed and Product streams.
- Size the Valve, Vessel, and Heat Exchange operations.

For this tutorial, the Session Preferences will be set so that the Dynamics Assistant will not manipulate the dynamic specifications.

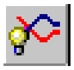
1. Open the **Tools** menu and select **Preferences**. The Session Preferences view appears.
2. Click the **Simulation** tab, then select the **Dynamics** page.
3. Ensure that the **Set dynamic stream specifications in the background** checkbox is cleared.

Figure 3.108



4. Close the Session Preference view, then close all open views on the UniSim Design desktop except for the PFD view.

   Next, you will initiate the Dynamics Assistant to evaluate the specifications required to run in dynamic simulation.

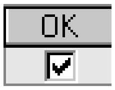


Dynamic Assistant icon

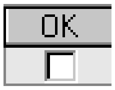
5. Click the **Dynamics Assistant** icon. Browse through each tab in the Dynamic Assistant view to inspect the recommendations.

   All recommendations in the Dynamic Assistant will be implemented by default unless you deactivate them. You can choose which recommendations will be executed by the Dynamic Assistant by activating or deactivating the OK checkboxes beside each recommendation.

Figure 3.109



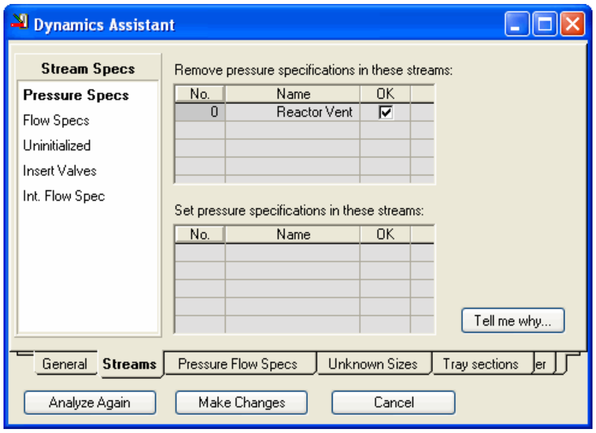
An **Active** recommendation will be implemented by the Dynamic Assistant.



An **Inactive** recommendation will not be implemented by the Dynamic Assistant.

6. Click the **Streams** tab. The Streams tab contains a list of recommendations regarding the setting or removing of pressure-flow specifications in the flowsheet.

Figure 3.110

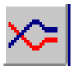


7. For each page in the **Streams** tab, activate or deactivate the following recommendations.

Page	Recommendation	Stream	OK Checkbox
Pressure Specs	**Remove Pressure Specifications**	Prop Oxide	Active
Flow Specs	**Remove Flow Specifications**	Prop Oxide	Active
		Water Feed	Active
Insert Valves	**Insert Valves**	Prop Oxide	Active
		Reactor Prods	Active
		Reactor Vent	Inactive
		Water Feed	Active

The Dynamics Assistant will insert valves on all the boundary flow streams except the Reactor Vent stream. This recommendation was deactivated since it is assumed that the CSTR reactor is exposed to the open air. Therefore, the pressure of the reactor is constant. A constant pressure can be modeled in the CSTR reactor by setting the Reactor Vent stream with a pressure specification. A valve should not be inserted on this stream.

8. Click the **Make Changes** button once only. All the active suggestions in the Dynamics Assistant are implemented. Close the Dynamics Assistant view.



Dynamic Mode Icon

9. Switch to Dynamic mode by pressing the **Dynamic Mode** icon. When asked if you want to resolve the dynamics assistant items before moving into dynamics, click the **No** button.

   Since the suggestion to insert a valve on the Reactor Vent stream was deactivated, you must set a pressure specification on this

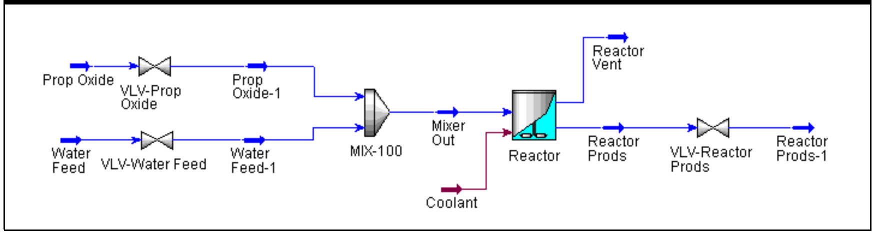
stream.

10. Double-click the Reactor Vent stream icon in the PFD. The property view appears.
11. Click the **Dynamics** tab, then select the **Specs** page.
12. In the Pressure Specification group, click in the **Active** checkbox to activate the specification.
13. Close the Reactor Vent stream property view.

> **In order for the CSTR to operate in steady state and dynamic mode, the vessel must be specified with a volume. Since the Dynamic Assistant detected that a volume was already specified for the CSTR reactor, it did not attempt to size it.**

14. The PFD for the dynamic tutorial (before the addition of the controllers) should look like the following figure.

Figure 3.111



15. Save the case as **DynTUT3-2.usc**.

3.3.3 Modeling a CSTR Open to the Atmosphere

The CSTR reactor is open to the atmosphere and the liquid level of the reactor can change in dynamic mode. This means that the vapour space in the liquid reactor also varies with the changing liquid level. In order to model this effect, the Reactor Vent stream was set with a constant pressure specification. However, one additional modification to the Reactor Vent stream is required.

Since the liquid level in the CSTR can move up and down, regular and reverse flow can be expected in the Reactor Vent stream. When vapour exits the reactor vessel (regular flow), the composition of the Reactor Vent stream is calculated from the existing vapour in the vessel. When vapour enters the vessel (reverse flow), the composition of the vapour stream from the atmosphere must be defined by the Product Block attached to the Reactor Vent stream. It is therefore necessary to specify the Product Block composition.

The original steady state Chemicals tutorial used a Fluid Package which did not include any inert gases. Therefore, it is now necessary to return to the Simulation Basis Manager and add the required components to the Fluid Package.

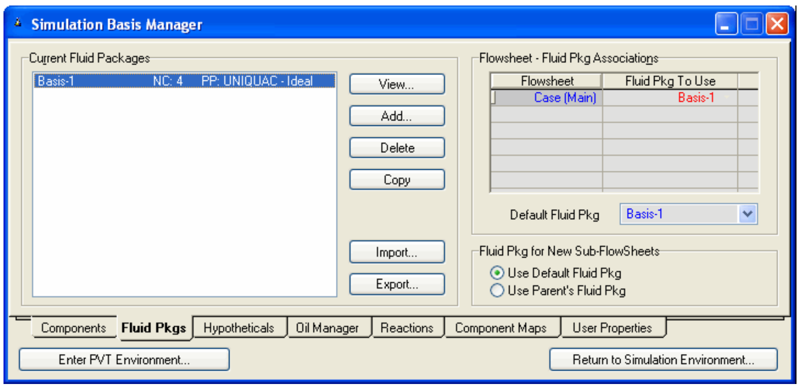
Enter Basis Environment icon

1. Click the **Enter Basis Environment** icon. The Simulation Basis Manager view appears.

   The Simulation Basis Manager allows you to create, modify, and otherwise manipulate Fluid Packages in the simulation case.

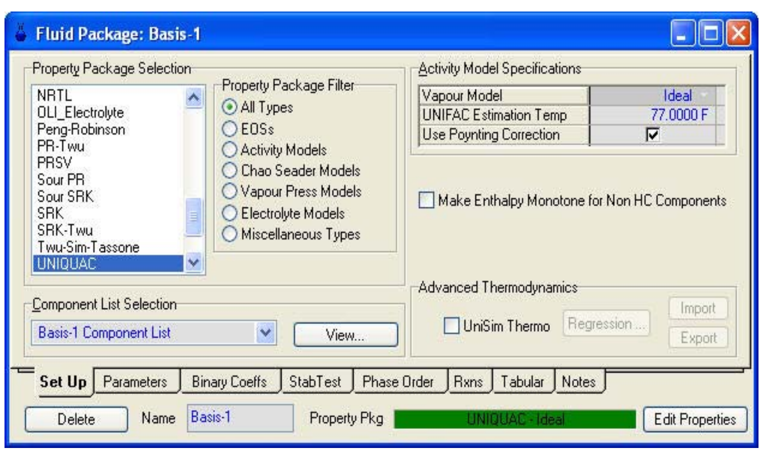
2. Click the **Fluid Pkgs** tab. In the Current Fluid Packages group, the Fluid Package associated with the Chemical Tutorial appears.

Figure 3.112



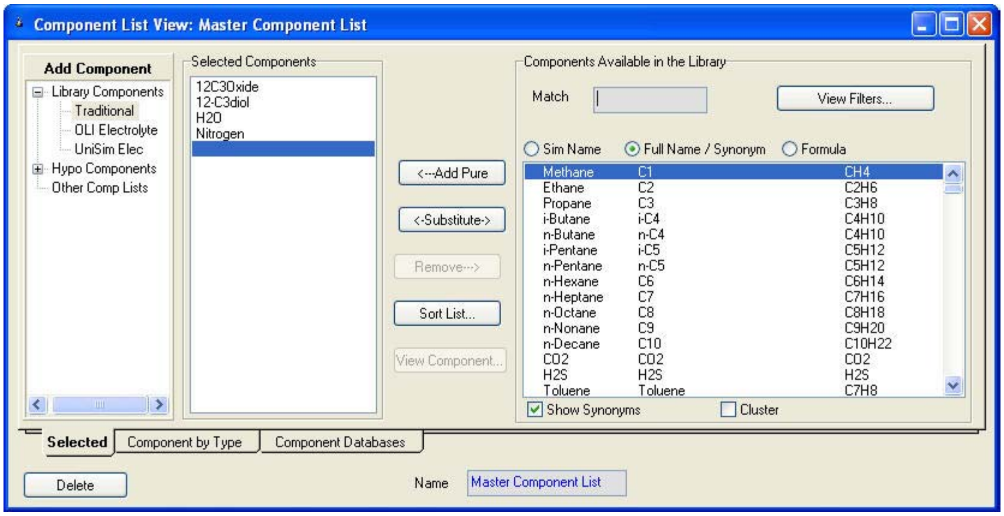
3. In the Current Fluid Packages group, select the fluid package, then click the **View** button. The Fluid Package: Basis-1 property view appears.

Figure 3.113

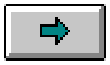


4. Click the **Set Up** tab. In the Component List Selection group, click the **View** button. The Component List View appears.

Figure 3.114



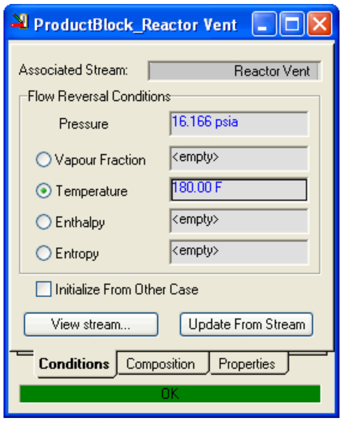
5. In the Components Available in the Component Library group, select the **Full Name/Synonym** radio button.
6. In the **Match** field, start typing Nitrogen. UniSim Design filters the component list to match your input.
7. When Nitrogen is selected in the list, press the **ENTER** key. Nitrogen is added to the Selected Components list. Close the Component List View.
8. Close the Fluid Package: Basis-1 property view.
9. In the Simulation Basis Manager view, click on the **Return to Simulation Environment** button. Answer **Yes** to the prompt that comes up.
10. On the PFD, double-click the Reactor Vent stream icon to open its property view.



View Downstream Operation icon

11. Click the **Product Block** button or the **View Downstream Operation** icon. The ProductBlock view appears.

Figure 3.115



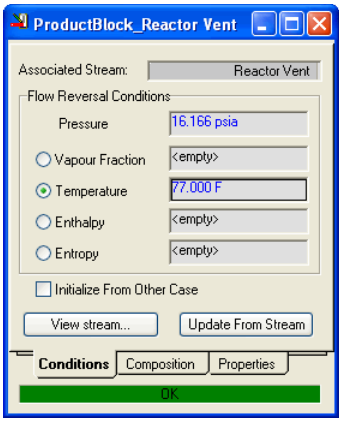
12. Click the **Composition** tab.
13. In the Compositions table, specify the composition of the reverse flow stream as follows:

Component	Mole Fraction
12C3Oxide	0.0
12-C3diol	0.0
H2O	0.0
Nitrogen	1.0

14. Click the **Conditions** tab.
15. In the Flow Reversal Conditions group, select the **Temperature** radio button.

16. In the field beside the Temperature radio button, enter 77°F. These stream conditions will be used to flash the pure nitrogen stream when the Reactor Vent flow reverses.

Figure 3.116



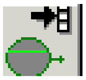
17. Close the ProductBlock_Reactor Vent view.
18. Close the Reactor Vent stream property view.
19. Save the case as **DynTUT3-3.usc**.

3.3.4 Adding Controller Operations

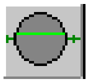
In this section you will identify and implement key control loops using PID Controller logical operations. Although these controllers are not required to run in dynamic mode, they will increase the realism of the model and provide more stability.

Level Control

First you will install a level controller to control the liquid level in the CSTR Reactor operation.



Control Ops icon

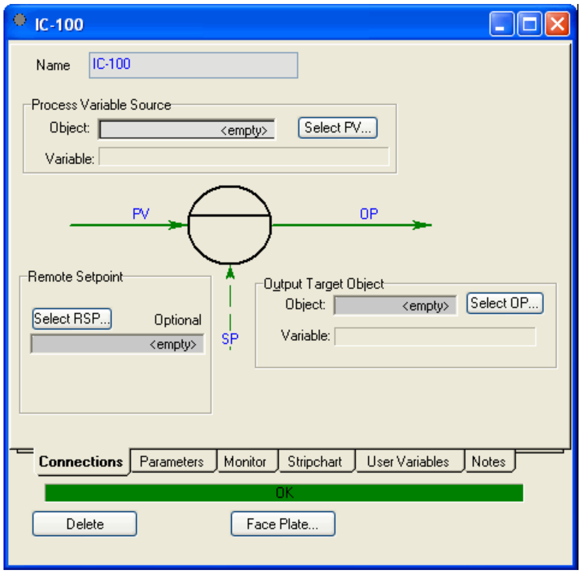


PID Controller icon

1. Press **F4** to activate the Object Palette, if required.
2. In the Object Palette, click the **Control Ops** icon. A sub-palette appears.
3. In the sub-palette, click the **PID Controller** icon. The cursor changes to include a frame and a + sign.
4. In the PFD, click near the Reactor icon. The IC-100 icon appears. This controller will serve as the Reactor level controller.

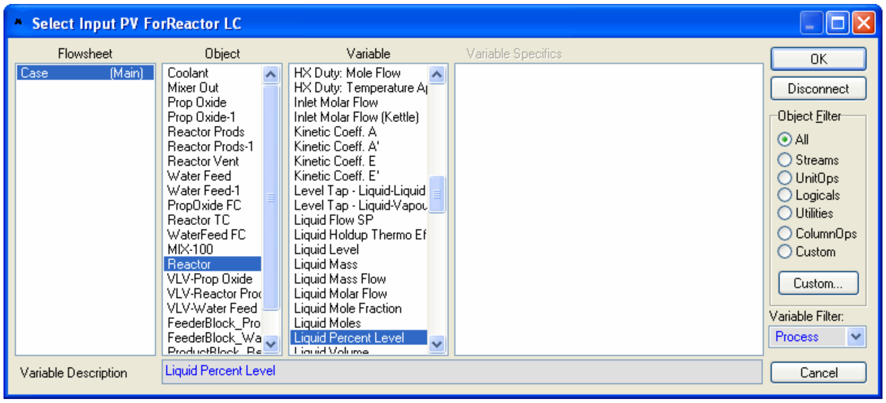
5. Double-click the IC-100 icon. The controller's property view appears.

Figure 3.117



6. In the **Connections** tab, click in the **Name** field and change the name to **Reactor LC**.
7. In the Process Variable Source group, click the **Select PV** button. The Select Input PV view appears.
8. In the Object group list, select **Reactor**.
9. In the Variable list, select **Liquid Percent Level**.

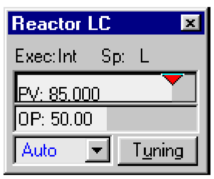
Figure 3.118



10. Click the **OK** button.
11. In the Output Target Object group, click the **Select OP** button. The Select OP Object view appears.

12. In the Object list, select **VLV-Reactor Prods**.
13. In the Variable list, select **Actuator Desired Position**, then click the **OK** button.
14. In the Reactor LC view, click the **Parameters** tab, then select the **Configuration** page.
15. On this page, enter the following information:

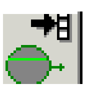
In this cell...	Enter...
Action	Direct
Kc	2
Ti	10 minutes
PV Minimum	0%
PV Maximum	100%



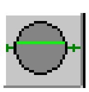
16. Click the **Face Plate** button at the bottom of the property view. The Reactor LC face plate view appears.
17. From the drop-down list, select Auto to change the controller mode.
18. Double-click in the **PV** value field, type 85, then press **ENTER**.
19. Close the Reactor LC face plate view, then close the Reactor LC property view.

Flow Control

Next you will add flow controllers to the feed streams in the process.



Control Ops icon



PID Controller icon

1. The Control Ops sub-palette should still be open. If it isn't, click the **Control Ops** icon in the Object Palette.
2. In the sub-palette, click the **PID Controller** icon.
3. In the PFD, click above the Prop Oxide stream icon. The IC-100 icon appears. This controller will serve as the Prop Oxide flow controller.
4. Double-click the IC-100 icon to open its property view.
5. Specify the following details:

Tab [Page]	In this cell...	Enter...
Connections	Name	PropOxide FC
	Process Variable Source	Prop Oxide, Mass Flow
	Output Target Object	VLV-Prop Oxide, Actuator Desired Position
Parameters [Configuration]	Action	Reverse
	Kc	0.1
	Ti	5 minutes
	PV Minimum	0 lb/hr
	PV Maximum	18,000 lb/hr

6. Click the **Face Plate** button. Change the controller mode to Auto, and input a set point of 8712 lb/hr.
7. Close the PropOxide FC face plate view and property view.
8. In the Object sub-palette, click the **PID Controller** icon.
9. In the PFD, click below the Water Feed stream icon. The controller icon appears. This controller will serve as the Water Feed flow controller.
10. Double-click the controller icon, then specify the following details:

Tab [Page]	In this cell...	Enter...
Connections	Name	WaterFeed FC
	Process Variable Source	Water Feed, Mass Flow
	Output Target Object	VLV-Water Feed Actuator Desired Position
Parameters [Configuration]	Action	Reverse
	Kc	0.1
	Ti	5 minutes
	PV Minimum	0 lb/hr
	PV Maximum	22,000 lb/hr

11. Click the **Face Plate** button. Change the controller mode to Auto and input a set point of 11,000 lb/hr.
12. Close the WaterFeed FC face plate view and property view.

Temperature Control

Next you will install temperature controller to control the temperature of the CSTR reactor. The control will be implemented using an energy utility stream.

1. In the Object sub-palette, click the **PID Controller** icon, then click in the PFD above and to the left of the Reactor icon.

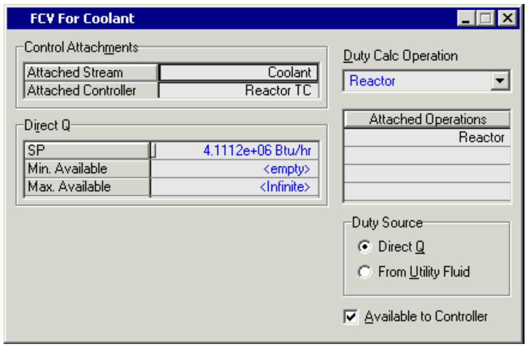
   The controller icon appears. This controller will serve as the Reactor temperature controller.
2. Double-click the controller icon, then specify the following details.

Tab [Page]	In this cell...	Enter...
Connections	Name	Reactor TC
	Process Variable Source	Reactor, Vessel Temperature
	Output Target Object	Coolant Control Valve

Tab [Page]	In this cell...	Enter...
Parameters [Configuration]	Action	Direct
	Kc	1.75
	Ti	5 minutes
	PV Minimum	70°F
	PV Maximum	300°F

3. Click the **Control Valve** button. The FCV for Coolant view appears.

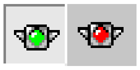
Figure 3.119



4. In the Duty Source group, select the **Direct Q** radio button.
5. In the Direct Q group table, enter the following information

In this cell...	Enter...
Minimum Available	0 Btu/hr
Maximum Available	1 x 10^7 Btu/hr

6. Close the FCV for Coolant view.
7. Click the **Face Plate** button. Change the controller mode to Auto and input a set point of 140°F.
8. Close the Reactor TC face plate view and property view.
9. Save the case as **DynTUT3-4.usc**.

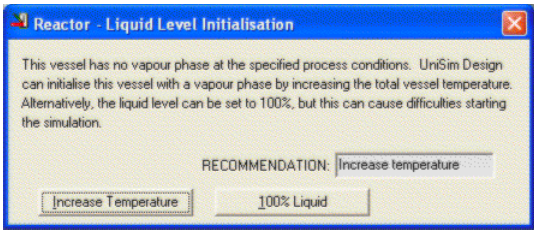


Integrator icons
Green=Active
Red=Holding

10. The integrator can be run at this point. Click the **Integrator Active** icon in the tool bar.
11. When you are given the option to run the dynamic assistant first before running the integrator, click the **No** button.

    When the integrator is initially run, UniSim Design will detect that the Reactor does not have a vapour phase at the specified process conditions. You have the option to select either the default, which is to Increase Temperature, or choose 100% Liquid in the Reactor.

Figure 3.120



12. Select the default setting, which is **Increase Temperature**.
13. Let the integrator run for a while, then click the **Integrator Holding** icon to stop the Integrator.

    At this point you can make changes to key variables in the process then observe the changes in the dynamic behaviour of the model.

    Next you will monitor important variables in dynamics using strip charts.

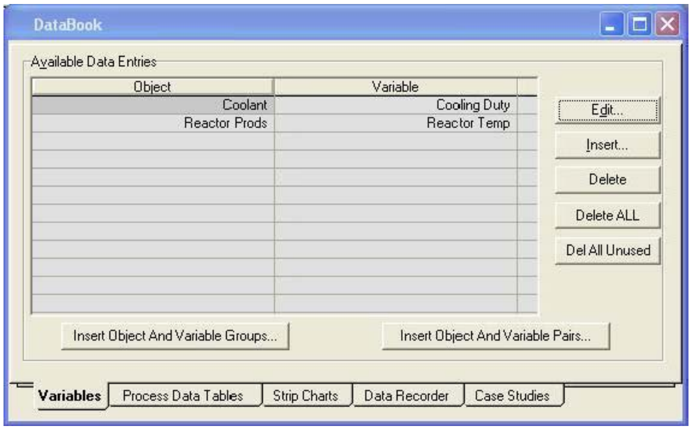
3.3.5 Monitoring in Dynamics

Now that the model is ready to run in dynamic mode, you will create a strip chart to monitor the general trends of key variables.

Add all of the variables that you would like to manipulate or model. Include feed and energy streams that you want to modify in the dynamic simulation.

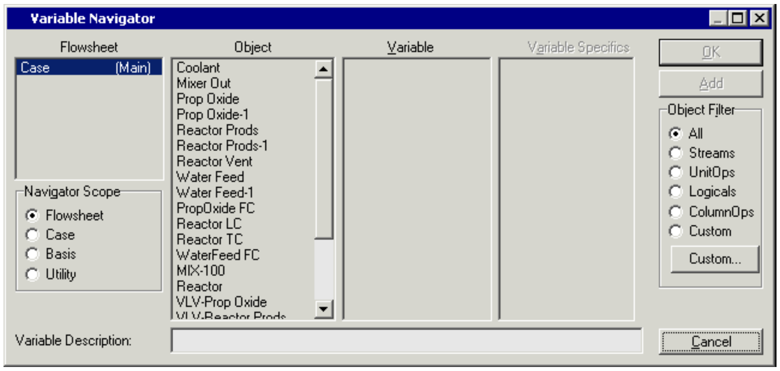
1. Open the Databook by using the hot key combination **CTRL D**. The following is a general procedure to install strip charts in UniSim Design.

Figure 3.121



2. On the **Variables** tab, click on the **Insert** button. The Variable Navigator appears.

Figure 3.122



Select the Flowsheet, Object, and Variable for any of the suggested variables. For Reactor Prods also select the Variable Specifics indicated.

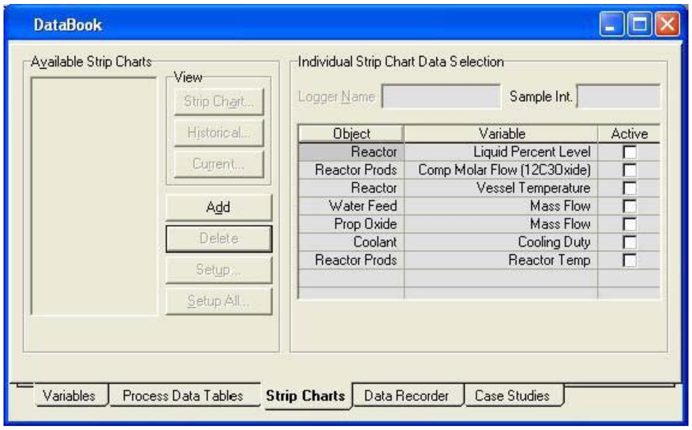
See the tables below for a list of suggested variables:

Variables to Manipulate	
Object	**Variable**
Prop Oxide	Mass Flow
Water Feed	Mass Flow

Variables to Monitor		
Object	**Variable**	**Variable Specifics**
Reactor	Vessel Temperature	
Reactor Prods	Comp Molar Flow	12C3Oxide
Reactor	Liquid Percent Level	

3. Click on the **OK** button to return to the Databook. The variable will now appear on the **Variables** tab.
4. Repeat the procedure to add all remaining variables to the Databook.
5. Click the **Strip Charts** tab in the Databook view.

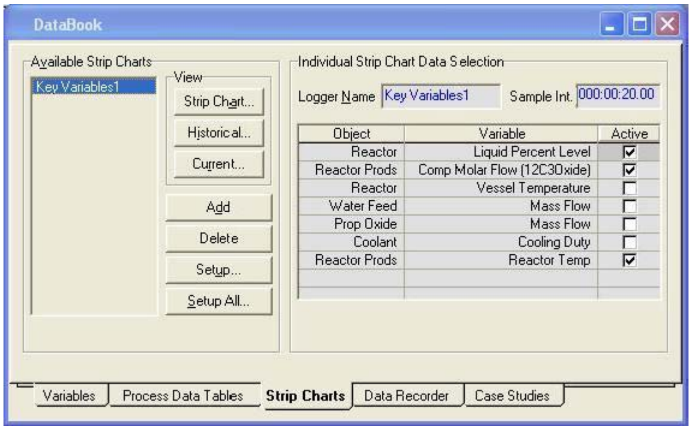
Figure 3.123



6. Click the **Add** button. UniSim Design will create a new strip chart with the default name DataLogger1.
7. In the **Logger Name** field, change the name to Key Variables1.

8. Click the **Active** checkbox for each of the variables that you would like to monitor. Keep the number of variables per Strip Chart to four or fewer, for easier viewing.

Figure 3.124



You can change the configuration of each strip chart by clicking the **Setup** button.

9. If required, add more strip charts.
10. Click the **Strip Chart** button to view each strip chart.

    To view a legend for the Strip Chart variables, right-click inside the Strip Chart view and select **Legend** from the menu.

    You can also maximize/resize the Strip Chart views to see the details.
11. Click the **Start Integrator** icon and observe as the variables line out. If you see a warning regarding the Dynamics Assistant, click the **No** button.

    When you are finished, click the **Integrator Holding** icon to stop the integrator.
12. At this point you can manipulate various variables within the design and observe the response of other variables.

B UniSim Design Applications

This section contains examples that illustrate many of the features in UniSim Design. The applications include aspects of Conceptual Design, Steady State modeling, and Optimization. All aspects are not illustrated in every example, so the areas of interest in each application are highlighted in the sections below.

The UniSim Design Applications describe, in general terms, how to completely model particular processes using various features of UniSim Design—detailed methods of constructing the models are not provided. If you require detailed descriptions on how to construct models in UniSim Design, see the comprehensive Tutorial section of this guide.

The examples in the Applications section provide a broad range of problems related to various segments of industry and are organized as follows.

Gas Processing

G1 Acid Gas Sweetening with DEA – Steady State Modeling, Optional Amines Package

The Amines Property Package is an optional property package. It is not included in the base version of UniSim Design. Contact Honeywell for more information, or e-mail us at **info@unisim.support@ honeywell.com**.

A sour natural gas stream is stripped of H2S and CO2 in a Contactor (absorber) tower. The rich DEA (diethanolamine) is regenerated in a Stripping tower and the lean DEA is recycled back to the Contactor. To solve this example, you must have the Amines property package, which is an optional property package. A spreadsheet is used to calculate various loadings and verify that they are within an acceptable range.

Refining

R1 Atmospheric Crude Tower – Steady State Modeling, Oil Characterization

A preheated (450°F) light crude (29 API) is processed in an atmospheric fractionation tower to produce naphtha, kerosene, diesel, atmospheric gas oil (AGO) and atmospheric residue products. A complete oil characterization procedure is part of this example application.

R2 Sour Water Stripper – Steady State Modeling, Sour Thermo Options, Case Study

Sour water is fed to a distillation tower for NH_3 and H_2S removal. The use of the Sour Peng Robinson (Sour_PR) is highlighted. UniSim Design's built-in Case Study tool is used to examine the effects of varying column feed temperatures.

Petrochemicals

P1 Propane/Propylene Splitter – Steady State Modeling, Column Sub-flowsheet

The individual Stripper tower and Rectifier tower components of a propane/propylene splitter system are modeled. Two separate towers in the same Column sub-flowsheet are used in this example to illustrate the simultaneous solution power of UniSim Design's Column sub-flowsheet.

Chemicals

C1 Ethanol Plant – Steady State Modeling

An ethanol production process is modeled right from the fermentor outlet through to the production of low grade and high grade (azeotropic) ethanol products.

C2 Synthesis Gas Production – Steady State Modeling, Reaction Manager, Reactors

Synthesis gas (H_2/N_2 on a 3:1 basis) is the necessary feedstock for an ammonia plant. The traditional process for creating synthesis gas is explored in this example. Air, steam, and natural gas are fed to a series of reactors, which produces a stoichiomtrically correct product. Extensive use of UniSim Design's Reaction Manager is illustrated as four individual reactions are grouped into three reaction sets that are used in five different reactors. This example also demonstrates the use of an Adjust operation to control a reactor outlet temperature. The case is then converted to a dynamics simulation by adding valves and assigning pressure flow specifications on the boundary streams. Reactors are sized using the actual gas flow and the residence time. A spreadsheet operation imports the H_2/N_2 molar ratio to a ratio controller, controlling the Air flowrate. Temperature controllers are used to achieve the reactors setpoint by manipulating the duty streams.

UniSim Design Extensibility

X1 Case Linking – Steady State Modeling

This case explores the use of the User Unit Operation to link two UniSim Design simulation cases such that the changes made to the first case are automatically and transparently propagated to the second case. Within each User Unit Op, two Visual Basic macros are used. The **Initialize()** macro sets the field names for the various stream feed and product connections and created two text user variables. The **Execute()** macro uses the **GetObject** method to open the target link case and then it attempts to locate the material stream, in the target case, named by the Initialize() macro.

G1 Acid Gas Sweetening with DEA

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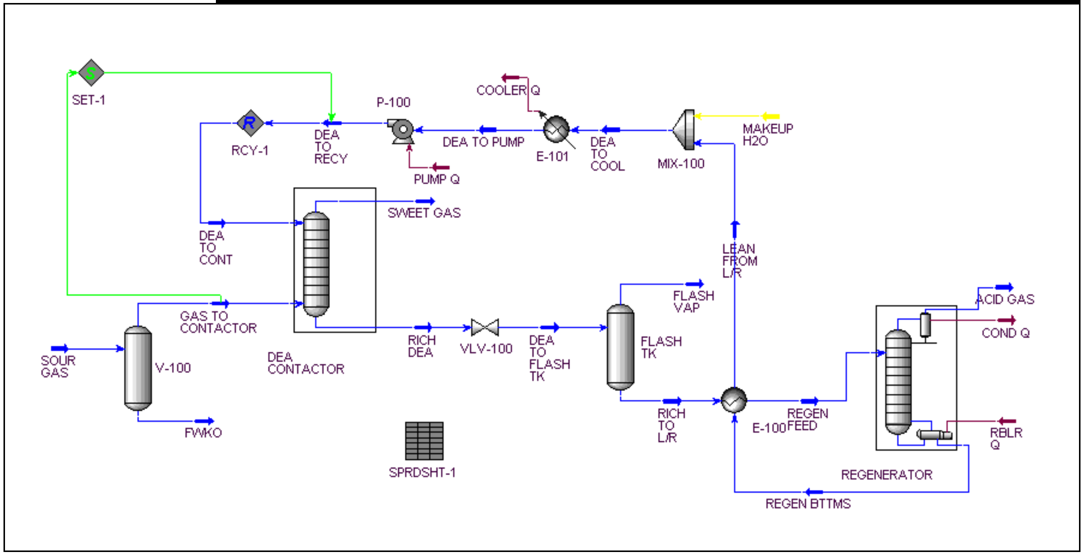
G1.1 Process Description

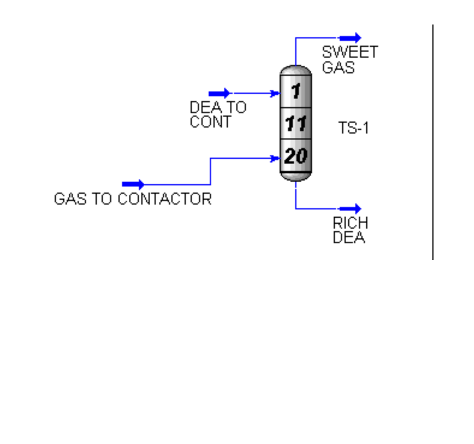
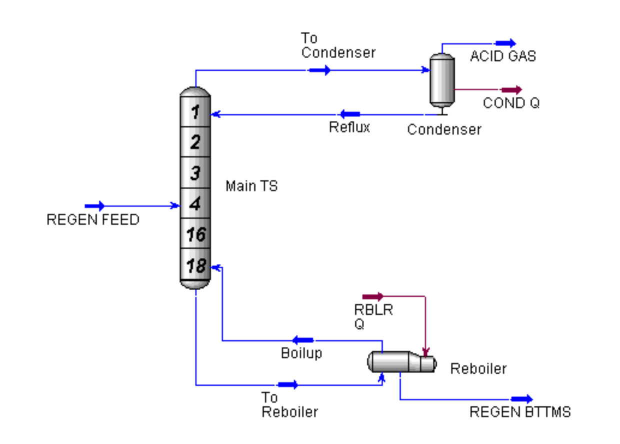
In this example, a typical acid gas treating facility is simulated. A water-saturated natural gas stream is fed to an amine contactor. For this example, Diethanolamine (DEA) at a strength of 28 wt% in water is used as the absorbing medium. The contactor consists of 20 real stages. The rich amine is flashed from the contactor pressure of 1000 psia to 90 psia to release most of the absorbed hydrocarbon gas before it enters the lean/rich amine exchanger. In the lean/rich exchanger, the rich amine is heated to a regenerator feed temperature of 200°F. The regenerator also consists of 20 real stages. Acid gas is rejected from the regenerator at 120°F, while the lean amine is produced at approximately 255°F. The lean amine is cooled and recycled back to the contactor.

Figure G1.1



Recommended amine strength ranges:

Lean Amine Strength in Water	
Amine	**Wt%**
MEA	15-20
DEA	25-35
TEA, MDEA	35-50
DGA	45-65

Figure G1.2	Figure G1.3
	

There are three basic steps used in modeling this process:

1. **Setup**. The component list includes **C1** through **C7** as well as **N2**, **CO2**, **H2S**, **H2O** and **DEA**.
2. **Steady State Simulation**. The case will consist of an absorber scrubbing the inlet gas using a DEA solution, which will be regenerated in a distillation column. Sweet gas will leave the top of the absorber, whereas the rich amine stream from the bottom will be sent to a regenerator column. An analysis on both the **SWEET GAS** and the **ACID GAS** will be performed to satisfy the specified criterion.
3. **Dynamics Simulation**. The steady state solution will be used to size all the unit operations and tray sections. An appropriate control strategy will be implemented and the key variables will be displayed.

G1.2 Setup

The Amines property package has a limit temperature range. So during the construction of the simulation/flowsheet, some streams will appear yellow in colour. A warning view will also appear to warn you that the stream has exceeded the temperature range.

For this application, you can ignore these warnings.

1. In the Session Preferences view, clone the **Field** unit set.
2. Change the default units for the **Liquid Volume Flow** to **USGPM** for the cloned unit set.
3. In the Component List view, select the following components: **N2**, **CO2**, **H2S**, **C1**, **C2**, **C3**, **i-C4**, **n-C4**, **i-C5**, **n-C5**, **C6**, **C7**, **H2O**, and **DEAmine**.
4. In the Fluid Package view, select the following property package: **Amines**.

   The Amines property package is required to run this example problem. This is a D.B. Robinson proprietary property package that predicts the behaviour of amine-hydrocarbon-water systems.
5. Use the Li-Mather/Non-Ideal Thermodynamic model.

G1.3 Steady State Simulation

There are two main steps for setting up this case in steady state:

1. **Installing the DEA Contractor**. A 20 stage absorber column will be used to scrub the SOUR GAS stream with DEA solution (DEA TO CONT). The SWEET GAS will leave the tower from the top whereas the pollutant rich liquid will be flashed before entering the REGENERATOR.
2. **Regenerating the DEA**. The liquid stream from the absorber will be regenerated in a 18 tray distillation column with a condenser and reboiler. The ACID GAS will be rejected from the top and the regenerated DEA will be send back to the DEA CONTACTOR.

G1.3.1 Installing the DEA CONTACTOR

Before the amine contactor can be solved, an estimate of the lean amine feed (DEA TO CONT) and the inlet gas stream (SOUR GAS) must be provided. The DEA TO CONT stream will be updated once the recycle operation is installed and has converged.

Add Feed Streams

Define the following material streams:

DEA to Cont uses Mass fractions; Sour Gas uses Mole fractions.

DEA TO CONT material stream	
In this cell...	**Enter...**
Name	DEA TO CONT
Temperature	95 F
Pressure	995 psia
Std Ideal Liq Vol Flow	190 USGPM
CO2 Mass Frac.	0.0018
Water Mass Frac.	0.7187
DEA Mass Frac.	0.2795

SOUR GAS material stream	
In this cell...	**Enter...**
Name	SOUR GAS
Temperature	86.0000 F
Pressure	1000.0000 psia
Molar Flow	25 MMSCFD
N2 Mole Frac.	0.0016
CO2 Mole Frac.	0.0413

SOUR GAS material stream	
H2S Mole Frac.	0.0172
C1 Mole Frac.	0.8692
C2 Mole Frac.	0.0393
C3 Mole Frac.	0.0093
iC4 Mole Frac.	0.0026
nC4 Mole Frac.	0.0029
iC5 Mole Frac.	0.0014
nC5 Mole Frac.	0.0012
nC6 Mole Frac.	0.0018
nC7 Mole Frac.	0.0072
H2O Mole Frac.	0.005
DEAmine Mole Frac.	0.000

Add a Separator

Any free water carried with the gas is first removed in a separator operation (V-100). Add and define the following separator operation:

Separator [V-100]		
Tab [Page]	**In this cell...**	**Enter...**
Design [Connections]	Inlets	SOUR GAS
	Vapour Outlet	GAS TO CONTACTOR
	Liquid Outlet	FWKO
Design [Parameters]	Pressure drop	0 psi

Add an Absorber Column

The Amines property package requires that real trays be modeled in the contactor and regenerator operations, but in order to simulate this, component specific efficiencies are required for H2S and CO2 on a tray by tray basis. These proprietary efficiency calculations are provided in the column as part of the Amines package. Tray dimensions must be supplied to enable this feature.

Before installing the column, ensure that the **Use Input Experts** checkbox is checked (from the Session Preferences view, Simulation tab, Options page).

1. Install an Absorber column operation with the specifications shown

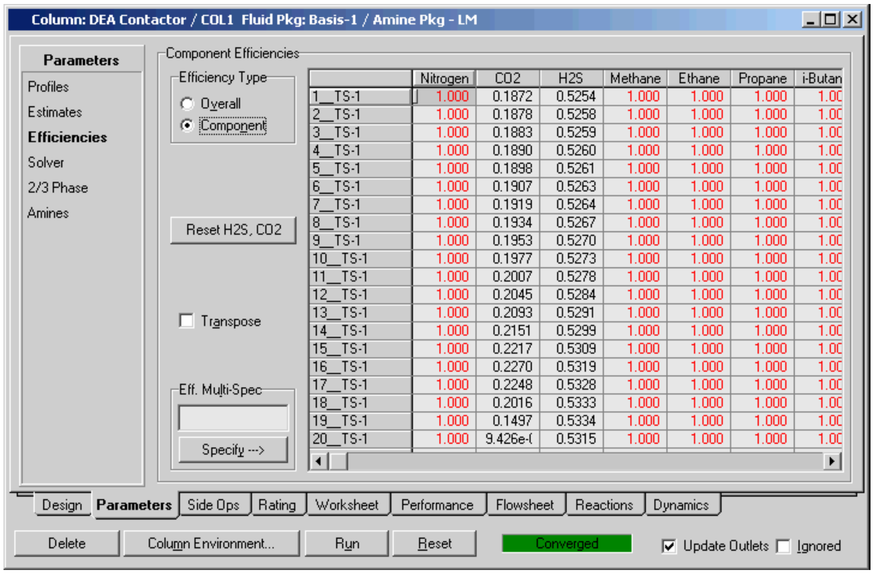
below.

Absorber Column [DEA CONTACTOR]		
Page	**In this cell...**	**Enter...**
Connections	No. of Stages	20
	Top Stage Inlet	DEA TO CONT
	Bottom Stage Inlet	GAS TO CONTACTOR
	Ovhd Vapour Outlet	SWEET GAS
	Bottoms Liquid Outlet	RICH DEA
Pressure Profile	Top	995 psia
	Bottom	1000 psia
Temperature Estimates	Top Temperature	100 F
	Bottom Temperature	160 F

Using the above information, the component specific tray efficiencies can be calculated.

2. Run the Column.
3. Once it has converged, click the **Parameters** tab and select the **Efficiencies** page.
4. Click the **Component** radio button and note the efficiency values for CO2 and H2S on each tray. UniSim Design provides an estimate of the component tray efficiencies but allows you to specify the individual efficiencies if required.

Figure G1.4



Next, add a valve and another separator.

Add a Valve

The stream Rich DEA from the absorber is directed to valve VLV-100, where the pressure is reduced to 90 psia; close to the regenerator operating pressure.

Valve [VLV-100]		
Tab [Page]	**In the cell...**	**Enter...**
Design [Connections]	Inlet	RICH DEA
	Outlet	DEA TO FLASH TK
Worksheet [Conditions]	Pressure (DEA TO FLASH TK)	90 psia

Add a Separator

Gases that are flashed off from the RICH DEA stream are removed using the rich amine flash tank (FLASH TK) which is modeled using a Separator operation.

Separator [FLASH TK]		
Tab [Page]	**In this cell...**	**Enter...**
Design [Connections]	Inlet	DEA TO FLASH TK
	Vapour Outlet	FLASH VAP
	Liquid Outlet	RICH TO L/R

G1.3.2 Regenerating the DEA

Add a Heat Exchanger

The stream RICH TO L/R is heated to 200°F (REGEN FEED) in the lean/ rich exchanger (E-100) prior to entering the regenerator, which is represented by a distillation column. Heat is supplied to release the acid gas components from the amine solution, thereby permitting the DEA to be recycled back to the contactor for reuse.

The heat exchanger is defined below.

Heat Exchanger [E-100]		
Tab [Page]	**In this cell...**	**Enter...**
Design [Connections]	Tube Side Inlet	RICH TO L/R
	Tube Side Outlet	REGEN FEED
	Shell Side Inlet	REGEN BTTMS
	Shell Side Outlet	LEAN FROM L/R

Heat Exchanger [E-100]		
Design [Parameters]	Tubeside Delta P	10 psi
	Shellside Delta P	10 psi
Rating [Sizing]	Tube Passes per Shell	1
Worksheet [Conditions]	Temperature (REGEN FEED)	200 F

Add a Distillation Column

The amine regenerator is modeled as a distillation column with 20 real stages - 18 stages in the Tray Section plus a Reboiler and Condenser.

1. Add a distillation column, configured as shown in the following table.

Distillation Column [Regenerator]		
Page	**In this cell...**	**Enter...**
Connections	No. of Stages	18
	Inlet Streams (Stage)	REGEN FEED (4)
	Condenser Type	Full Reflux
	Ovhd Vapour	ACID GAS
	Bottoms Liquid	REGEN BTTMS
	Reboiler Energy Stream	RBLR Q
	Condenser Energy Stream	COND Q
Pressure Profile	Condenser Pressure	27.5 psia
	Cond Pressure Drop	2.5 psi
	Reboiler Pres.	31.5 psia

For this tower, the component efficiencies will be fixed at 0.80 for H2S and 0.15 for CO2. The efficiencies of the condenser and reboiler must remain at 1.0, so enter the efficiencies for stages 1-18 only.

2. Select the **Component** radio button in the Efficiency Type group (**Parameters** tab, **Efficiencies** page), then click the **Reset H2S CO2** button.
3. Type the new efficiencies into the matrix.

Distillation Column [Regenerator]		
Tab [Page]	**In this cell...**	**Enter...**
Parameters [Efficiencies]	Condenser	1.0
	Reboiler	1.0
	1_TS to 18_TS CO2	0.15
	1_TS to 18_TS H2S	0.80
Parameters [Solver]	Damping Factor	0.40

4. Specify a **Damping Factor** of **0.40** (**Parameters** tab, **Solver** page) to provide a faster, more stable convergence.

5. Add two new column specifications, **Column Temperature** (called TTop) and **Column Duty** (called Reboiler Duty).
6. Set the default specifications as shown below.

Regenerator Specifications		
Tab [Page]	**In this cell...**	**Enter...**
Design [Specs]	Name Stage Spec Value	T Top Condenser 179.6 F
	Name Energy Stream Spec Value	Reboiler Duty RBLR Q@COL2 1.356e7 BTU/hr
	Name Stage Flow Basis Spec Value	Reflux Ratio Condenser Molar 0.5
	Name Draw Flow Basis Spec Value	Ovhd Vap Rate ACID GAS@COL2 Molar 2.0 MMSCFD

7. Delete the **Reflux Rate** and **REGEN Bttms Rate** specifications from the Column Specification list in the Column property view.
8. Set the **T Top** and **Reboiler Duty** specifications to Active; the Reflux Ratio and Ovhd Vap Rate specifications should be set as Estimates only.

   The reboiler duty is based on the guidelines provided below, which should provide an acceptable **H2S** and **CO2** loading in the lean amine.

Recommended Steam Rates lb Steam / USGAL Lean Amine (based on 1000 BTU / lb Steam)	
Primary Amine (e.g., MEA)	0.80
Secondary Amine (e.g., DEA)	1.00
Tertiary Amine (e.g., MDEA)	1.20
DGA	1.30

   Water make-up is necessary, since water will be lost in the absorber and regenerator overhead streams.

9. Install a Mixer operation to combine the lean amine from the regenerator with the MAKEUP H2O stream. These streams mix at the same pressure.
10. Define the composition of MAKEUP H2O as all water, and specify a temperature of 70°F and pressure of 21.5 psia. The flow rate of the total lean amine stream will be defined at the outlet of the mixer, and UniSim Design will calculate the required flow of makeup water.

11. Set the overall circulation rate of the amine solution by specifying a Standard Ideal Liquid Volume Flow of 190 USGPM in stream DEA TO COOL. UniSim Design will back-calculate the flow rate of makeup water required.

Mixer [MIX-100]		
Tab [Page]	**In this cell...**	**Enter...**
Design [Connections]	Inlets	MAKEUP H2O
		LEAN FROM L/R
	Outlet	DEA TO COOL
Design [Parameters]	Automatic Pressure Assignment	Set Outlet to Lowest Inlet
Worksheet [Conditions]	Temperature (MAKEUP H2O)	70 F
	Pressure (MAKEUP H2O)	21.5 psia
	Std Liq Vol Flow (DEA to Cool)	190.5 USGPM
Worksheet [Composition]	H2O Mass Frac. (MAKEUP H2O)	1.0

When you have finished specifying the DEA TO COOL stream you will receive a warning message stating that the temperature of the Makeup H2O stream exceeds the range of the property package and the stream will turn yellow. Since there is no DEA present in this stream, the warning can be ignored without negatively affecting the results of this case.

Add a Cooler

The Cooler operation will remain unconverged until the Set operation has been installed.

Add a cooler and define it as indicated below. Cooler E-101 cools the lean DEA on its way to the main pump.

Cooler [E-101]		
Tab [Page]	**In this cell...**	**Enter...**
Design [Connections]	Inlet	DEA TO COOL
	Outlet	DEA TO PUMP
	Energy Stream	COOLER Q
Design [Parameters]	Delta P	5 psi

Add a Pump

The Pump operation will remain unconverged until the Set operation has been installed.

Add a pump and define it as indicated below. Pump P-100 transfers the

regenerated DEA to the Contactor.

Pump [P-100]		
Tab [Page]	**In this cell...**	**Enter...**
Design [Connections]	Inlet	DEA TO PUMP
	Outlet	DEA TO RECY
	Energy	PUMP Q
Worksheet [Conditions]	Temperature [F] (DEA TO RECY)	95°F

Add a Set Operation

Install a Set operation (SET-1) to maintain the pressure of stream DEA TO RECY at 5 psi lower than the pressure of the gas feed to the absorber.

Set [SET-1]		
Tab [Page]	**In this cell...**	**Enter...**
Connections	Target	DEA TO RECY
	Target Variable	Pressure
	Source	GAS TO CONTACTOR
Parameters	Multiplier	1
	Offset	-5

Add a Recycle Operation

A Recycle operation is installed with the fully defined stream DEA TO RECY as the inlet and DEA TO CONT as the outlet. The lean amine stream, which was originally estimated, will be replaced with the new, calculated lean amine stream and the contactor and regenerator will be run until the recycle loop converges.

To ensure an accurate solution, reduce the sensitivities for flow and composition as indicated below.

Recycle [RCY-1]		
Tab [Page]	**In this cell...**	**Enter...**
Connections	Inlet	DEA TO RECY
	Outlet	DEA TO CONT
Parameters [Variables]	Flow	1.0
	Composition	0.1

G1.4 Simulation Analysis

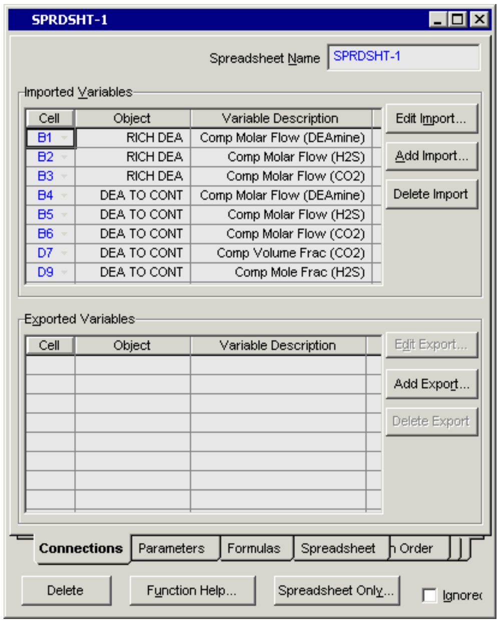
The incoming sour gas contains 4.1% CO_2 and 1.7% H_2S. For an inlet gas flow rate of 25 MMSCFD, a circulating solution of approximately 28 wt.% DEA in water removes virtually all of the H_2S and most of the CO_2. A typical pipeline specification for the sweet gas is no more than 2.0 vol.% CO_2 and 4 ppm (volume) H_2S. If you look at the property view of the Sweet Gas stream you will see the sweet gas produced easily meets these criteria.

G1.5 Calculating Lean & Rich Loadings

Concentrations of acid gas components in an amine stream are typically expressed in terms of amine loading—defined as moles of the particular acid gas divided by moles of the circulating amine. The Spreadsheet in UniSim Design is well-suited for this calculation. Not only can the loading be directly calculated and displayed, but it can be incorporated into the simulation to provide a “control point” for optimizing the amine simulation. Also for convenience, the CO_2 and H_2S volume compositions for the Sweet Gas stream are calculated.

The following variables are used for the loading calculations.

Figure G1.5



The following formulas will produce the desired calculations.

Figure G1.6

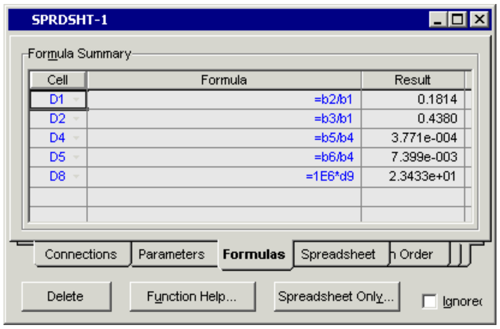
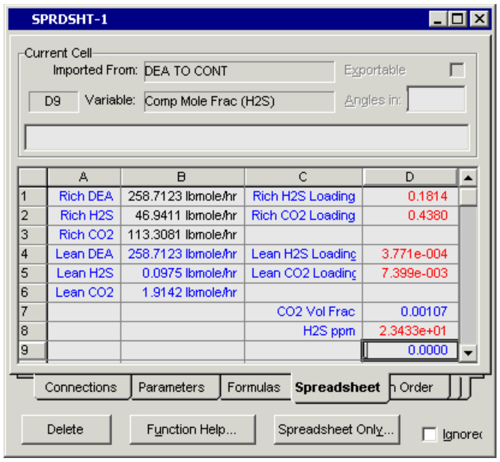


Figure G1.7



The acid gas loadings can be compared to values recommended by D.B. Robinson as shown below.

Maximum Acid Gas Loadings (moles acid gas/mole of amine)		
	CO2	**H2S**
MEA, DGA	0.5	0.35
DEA	0.45	0.30
TEA, MDEA	0.30	0.20

G1.6 Dynamic Simulation

The Amines property package used in this application has a limit temperature range. So when a stream exceeds the temperature range, a warning view will appear and the stream becomes yellow in colour.

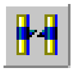
For this application, you can ignore this warning.

In the second part of the application, the steady state case will be converted into dynamics. The general steps that will be used to navigate through this detailed procedure are as follows:

1. **Converting from Steady State**. To prepare the case for dynamic simulation, valves will be installed to define pressure flow relations and PF specifications will be added to selected streams. The tray sizing utility will be implemented for sizing tray sections; all other unit operations will be sized.
2. **Adding Controllers**. In this step, appropriate controllers will be installed and defined manually.
3. **Preparing the Dynamics Simulation**. In the last step, the Databook will be set up. Changes will be made to key variables in the process and the dynamic behaviour of the model will be observed.

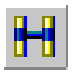
G1.6.1 Converting from Steady State

Changing the PFD



Break Connection icon

Use the **Break Connection** icon to break the connection between streams and unit operations.



Attach Mode icon

Use the **Attach Mode** icon to reconnect them.

A few changes will have to be made to the PFD in order to operate in Dynamic mode.

1. Delete the **Set-1** unit operation.
2. Set the pressure of the DEA TO RECY stream to **995** psia.
3. Install a Recycle operation between the REGEN BTTMS stream and the E-100 exchanger.

Recycle	**RCY-2**	
Page	**In this cell...**	**Enter...**
Connections	Inlet	REGEN BTTMS
	Outlet	REGEN BTTMS TO L/R

The Recycle operation only functions in Steady State mode. Its sole purpose in this case is to provide a suitable solution before entering Dynamic mode.

4. Delete the Std. Ideal Liq Vol Flow value in stream DEA TO COOL.
5. Specify the Std. Ideal Liq. Vol. Flow in stream MAKEUP H2O at 2.195 USGPM.
6. Delete MIX-100 and replace it with a tank, V-101. Name the vapour outlet from the tank Nitrogen Blanket.
7. Change the Heat Exchanger model of the E-100 exchanger from Exchanger Design (End Point) to Dynamic Rating. Delete the temperature of the REGEN FEED stream, since it will be calculated by the exchanger. Use the following table to set the new specifications for the exchanger.

Heat Exchanger	**E-100**	
Tab [Page]	**In this cell...**	**Enter...**
Design [Connections]	Shell Side Inlet	REGEN BTTMS TO L/R
Design [Parameters]	Heat Exchanger Model	Dynamic Rating
Rating [Parameters]	Model	Basic
	Overall UA	100270 Btu/F-hr

Add Pumps

Two pumps are added because Dynamics mode performs rating calculations that consider pressure differences and flow resistance. To accommodate this, you need to add equipment that significantly impacts the pressure and drives flow.

Add the following pumps to define the pressure flow relation.

Pump Name	**P-101**	
Tab [Page]	**In this cell...**	**Enter...**
Design [Connection]	Inlet	RICH TO PUMP
	Outlet	RICH TO VALVE
	Energy	Q-100
Design [Parameters]	Duty	3739.72 Btu/hr
Comments	Add this pump between the separator FLASH TK and the stream RICH to L/R.	

Pump Name	**P-102**	
Tab [Page]	**In this cell...**	**Enter...**
Design [Connection]	Inlet	REGEN BTTMS
	Outlet	REGEN BTTMS TO VALVE
	Energy	Q-101
Design [Parameters]	Power	1.972e5 Btu/hr
Comments	Add this pump between the stream REGEN BTTMS and the recycle RCY-2.	

Add Valves

1. Add the following valves to define the pressure flow relation.

Valve Name	**VLV-FWKO**	
Tab [Page]	**In this cell...**	**Enter...**
Design [Connection]	Inlet	FWKO
	Outlet	FWKO-1
Worksheet [Conditions]	Pressure (FWKO-1)	986.5 psia
Rating [Sizing]	Valve Opening	50%
	VLV-Flash Vap	
Tab [Page]	**In this cell...**	**Enter...**
Design [Connection]	Inlet	FLASH VAP
	Outlet	FLASH VAP-1
Worksheet [Conditions]	Pressure (Flash Vap-1)	89.99 psia
Rating [Sizing]	Valve Opening	50%
	VLV-101	
Tab [Page]	**In this cell...**	**Enter...**
Design [Connection]	Inlet	RICH TO VALVE
	Outlet	RICH TO L/R

Valve Name	VLV-FWKO	
Tab [Page]	**In this cell...**	**Enter...**
Design [Parameters]	Delta P	5.8 psi
Rating [Sizing]	Valve Opening	50%
Comments	Add this valve between the pump P-101 and the stream RICH TO L/R.	

Valve Name	VLV-102	
Tab [Page]	**In this cell...**	**Enter...**
Design [Connection]	Inlet	REGEN BTTMS TO VALVE
	Outlet	REGEN BTTMS-2
Design [Parameters]	Delta P	13.53 psi
Rating [Sizing]	Valve Opening	50%
Comments	Add this valve between the stream REGEN BTTMS TO VALVE and the recycle RCY-2.	
	VLV-103	
Tab [Page]	**In this cell...**	**Enter...**
Design [Connection]	Feed	DEA TO VALVE
	Product	DEA TO COOL
Design [Parameters]	Delta P	1 psi
Rating [Sizing]	Valve Opening	50%
Comments	Add this valve between V-101 and the stream DEA TO COOL.	
	VLV-100@COL1	
Tab [Page]	**In this cell...**	**Enter...**
Design [Connection]	Feed	1@COL1
	Product	SWEET GAS@COL1
Design [Parameters]	Delta P	1 psi
Rating [Sizing]	Valve Opening	50%
Comments	Add this valve between the vapour outlet of the absorber DEA Contactor and the stream SWEET GAS in the absorber sub-flowsheet.	
	VLV-100@COL2	
Tab [Page]	**In this cell...**	**Enter...**
Design [Connection]	Feed	2@COL2
	Product	ACID GAS@COL2
Design [Parameters]	Delta P	1 psi
Rating [Sizing]	Valve Opening	50%
Comments	Add this valve between the vapour outlet of the distillation column REGENERATOR and the stream ACID GAS in the Regenerator Column sub-flowsheet.	

For the Regenerator, you may need to click the **Reset** button before clicking the **Run** button to get the distillation column to solve.

Before proceeding any further, ensure that the case is completely solved.

2. Open the valves property view and move to the **Sizing** page of the **Rating** tab.
3. Select the **User Input** radio button and specify the Valve Opening as indicated.
4. Click the **Size Valve** button.
5. Repeat for all valves in the simulation.

Adding Pressure Flow Specifications

For more information regarding Pressure-Flow specifications in Column unit operations see **Chapter 8 - Column** in the **UniSim Design Operations Guide**.

In order to run the integrator successfully, the degrees of freedom for the flowsheet must be reduced to zero by setting the pressure-flow specifications. Normally, you would make one pressure-flow specification per flowsheet boundary stream, however, there are exceptions to the rule.

One extra pressure flow specification is required for the condenser attached to the column Regenerator. This rule applies only if there are no pieces of equipment attached to the reflux stream downstream of the condenser. Without other pieces of the equipment (i.e., pumps, coolers, valves) to define the pressure flow relation of these streams, they must be specified with a flow specification.

The pressure-flow specification can be activated in the **Dynamics** tab on the **Specs** page by selecting the **Active** checkbox. The steady state pressure-flow values should be used as a specification.

1. In the Main flowsheet, add the following pressure-flow specifications to the boundary streams.

Material Stream	Pressure Specification	Flow Specification	Value
SOUR GAS	Inactive	Molar Flow	25 MMSCFD
FWKO-1	Active	Inactive	986.5 psia
FLASH VAP-1	Active	Inactive	89.99 psia
MAKEUP H2O	Inactive	Ideal Liq Vol Flow	2.195 USGPM
SWEET GAS	Active	Inactive	994 psia
ACID GAS	Active	Inactive	26.5 psia
REFLUX@COL2	Inactive	Mass Flow	2983 lb/hr
Nitrogen Blanket	Active	Inactive	21.5 psia
DEA TO RECY	Inactive	Inactive	
DEA TO FLASH TK	Inactive	Inactive	

2. Ensure the **PF Relation** checkbox for all the valves is checked (**Dynamics** tab, **Specs** page).
3. Activate the **Efficiency** and **Power** checkboxes for pumps (you may have to deactivate the **Pressure Rise** checkbox).
4. On the E-100 property view, click the **Calculate K's** button (**Dynamics** tab, **Specs** page).

5. Deactivate the **Delta P** checkbox and select the **k** checkbox for both the Shell and Tube sides of E-100.
6. Also on the cooler E-101 property view, set the pressure flow option instead of the pressure drop by selecting the **Overall k Value** checkbox and deactivating the pressure drop checkbox.

Equipment Sizing

In preparation for dynamic operation, both column tray sections and the surrounding equipment must be sized. In steady state simulation, the column pressure drop is user specified. In dynamics, it is calculated using dynamic hydraulic calculations. Complications will arise in the transition from steady state to dynamics if the steady state pressure profile across the column is very different from that calculated by the Dynamic Pressure-Flow solver.

Column Tray Sizing

1. From the **Tools** menu, select **Utilities**. Add a Tray Sizing utility to size the DEA Contactor tray section.
2. Click the **Select TS** button. The Select Tray Section view appears.
3. From the Flowsheet list, select **DEA Contactor**.
4. From the Object list, select **TS-1**.
5. Click the **Auto Section** button to calculate the tray section dimension. Accept all the defaults.
6. Select the **Trayed** radio button in the Section Results group (**Performance** tab, **Results** page).
7. Confirm the following tray section parameters for Section_1.

Variable	Value
Section Diameter	3.5 ft
Weir Height	2 in
Tray Spacing	24 in
Weir Length	34.81 in
Number of Flow Paths	1

8. Calculate the Actual Weir Length using the Weir Length divided by the number of flow paths for the vapour.

Variable	Value
Actual Weir Length (Weir Length / 1)	34.81 in

9. Open the DEA Contactor column property view.
10. Click the **Rating** tab, then select the **Tray Sections** page.

11. Enter the tray section parameters for TS-1 obtained from the tray sizing utility.
12. Size the Regenerator tray section following the same procedure described above for the DEA Contactor. The Auto Section function may create two tray sections; ensure that the column is sized with only one tray section for all trays. Delete the section that does not match the specifications below.
13. Confirm the following tray section parameters for Main TS in the Regenerator:

Variable	Value
Section Diameter	3.5 ft
Weir Height	2 in
Tray Spacing	24 in
Total Weir Length	33.75 in
Number of Flow Paths	1
Actual Weir Length	33.75 in

14. In the Regenerator column property view, click the **Rating** tab, then select the **Tray Sections** page.
15. Enter the Section Diameter value shown above.

Vessel Sizing

The Condenser and Reboiler operations in the Regenerator column sub-flowsheet require proper sizing before they can operate effectively in Dynamics mode. The volumes of these vessel operations are determined using a 10 minute liquid residence time.

1. Open the Regenerator property view, then enter the Column Environment.
2. Open the Condenser property view.
3. Click the **Worksheet** tab, then select the **Conditions** page.
4. Confirm the following Std Ideal Liquid Volumetric Flow.

Stream	Std Ideal Liquid Volume Flow
Reflux	5.975 USGPM

5. Calculate the vessel volume as follows, assuming a 50% liquid level residence volume.

$$Vessel\ Volume\ =\ \frac{Total\ Liquid\ Exit\ Flow \cdot Residence\ Time}{0.5} \tag{G1.1}$$

6. Click the **Dynamics** tab, then select the **Specs** page.

7. In the Model Details group, specify the vessel volume as 15.97 ft^3 (as calculated with the above formula).
8. Specify the Level Calculator as a Horizontal cylinder.
9. Open the Reboiler property view.
10. Click the **Worksheet** tab, then select the **Conditions** page. Confirm the following Std Ideal Liquid Volume Flow.

Stream	Std Ideal Liquid Volume Flow
To Reboiler	239.7 bbl/day

11. Calculate the vessel volume using Equation **(G1.1)** and assuming a **50%** liquid level residence time.
12. Click the **Dynamics** tab, then select the **Specs** page.
13. In the Model Details group, specify the vessel volume as 641 ft^3 and the Level Calculator as a Horizontal cylinder.

Separator Sizing

The vapour flow rate through V-100 is large as compared to the liquid flow rate, therefore Separator V-100 is sized according to the terminal vapour velocity (Vertical Cylinder).

1. Use a residence time of 5 min and a 50% liquid level to size the separator FLASH TK.
2. Confirm the Std Ideal Liquid Volume flow in the table below and enter the vessel volume.
3. Click the **Rating** tab, then select the **Sizing** page. Select the Vertical orientation radio button for the separator.

Separator Name	FLASH TK	
Tab [Page]	**In this cell...**	**Enter...**
Worksheet [Conditions]	Std Liq Vol Flow (RICH TO PUMP)	498.27 USGPM
Rating [Sizing]	Volume	660 ft^3
	V-100	
Tab [Page]	**In this cell...**	**Enter...**
Rating [Sizing]	Diameter	5.94 ft
	Height	29.7 ft

Tank Sizing

The tank V-101 will be sized with a 10 minute liquid residence time and a **75%** liquid level. Confirm the volumetric flow rate of the exit stream

and specify the vessel volume (**Rating** tab, **Sizing** page).

Tank	**V-101**	
Tab [Page]	**In this cell...**	**Enter...**
Worksheet [Conditions]	LiqVol Flow (DEA TO VALVE)	194.4 USGPM
Rating [Sizing]	Volume	346.4 ft^3
Design [Parameters]	Liquid Level	75%

Heat Exchanger Sizing

The Shell and Tube heat exchanger E-100 will be sized with a 10 minute residence time for both the shell and the tube side (enter respective sizes on the **Rating** tab, **Parameters** page).

Heat Exchanger	**E-100**	
Tube Side Sizing		
Worksheet [Conditions]	Std Ideal Liq Vol Flow (RICH TO L/R)	498.27 USGPM
Rating [Parameters]	Volume	666 ft^3
Shell Side Sizing		
Worksheet [Conditions]	Std Ideal Liq Vol Flow (REGEN BTTMS TO L/R)	691.3 USGPM
Rating [Parameters]	Volume	925.2 ft^3

A 10 minute liquid residence time will also be used for sizing the cooler E-101 (**Dynamics** tab, **Specs** page).

Cooler	**E-101**	
Tab [Page]	**In this cell...**	**Enter...**
Worksheet [Conditions]	Std Ideal Liq Vol Flow (DEA TO COOL)	194.4 USGPM
Dynamics [Specs]	Volume	259.8 ft^3

Running the Integrator

1. Switch to the Dynamic mode by clicking the **Dynamic Mode** button. Click **No** when asked if you want the Dynamics Assistant to help you resolve items in Steady State before switching to Dynamic mode.
2. Open the Product Block for stream Nitrogen Blanket.
3. Ensure that the radio button for temperature is selected, and the value is specified as **70°F**.

4. Click the **Composition** tab and set the composition to **100% Nitrogen**.
5. Return to the **Conditions** tab, and press the **Export Conditions to Stream** button.
6. Open the Integrator view and change the **Step Size** to **0.2** sec on the **General** tab.
7. Click the **Options** tab and make sure that the **Singularity analysis before running** checkbox is selected.
8. Run the integrator for 2 minutes to ensure that the degrees of freedom for pressure flow specification is zero and all the vessels are sized. Select **Non-Equilibrium Vapour** when asked how you want to initialize V-101.

G1.6.2 Adding a Control Scheme

The following Controllers will be used in the Dynamics model:

- Level
- Temperature
- Pressure
- Flow

Level Controllers

Level Controller Name	V100-LC	
Tab [Page]	**In this cell...**	**Enter...**
Connections	Process Object	V-100
	Process Variable	Liquid Percent Level
	Output Variable	VLV-FWKO
Parameters [Configuration]	PVmin	0%
	PVmax	100%
	Action	Direct
	Mode	Auto
	SP	50%
	Kc	2
	Ti	2
	FLASH TK-LC	
Tab [Page]	**In this cell...**	**Enter...**
Connections	Process Object	FLASH TK
	Process Variable	Liquid Percent Level
	Output Variable	VLV-101
Parameters [Configuration]	PVmin	0%
	PVmax	100%
	Action	Direct
	Mode	Auto
	SP	50%
	Kc	2
	Ti	2

Level Controller Name	LIC-100	
Tab [Page]	**In this cell...**	**Enter...**
Connections	Process Object	V-101
	Process Variable	Liquid Percent Level
	Output Variable	MAKEUP H2O
To size the Control Valve for the MAKEUPH2O stream, select the *Control Valve* button.		
FCV for MAKEUP H2O	Flow Type	Mass Flow
	Min Available	0.0 lb/hr
	Max Available	1200 lb/hr
Parameters [Configuration]	PVmin	0%
	PVmax	100%
	Action	Reverse
	Mode	Auto
	SP	50%
	Kc	2
	Ti	2

Level Controller Name	**LIC-100**	
	Reb-LC@COL2	
Tab [Page]	**In this cell...**	**Enter...**
Connections	Process Object	Reboiler@COL2
	Process Variable	Liquid Percent Level
	Output Variable	VLV-102@Main
Parameters [Configuration]	PVmin	0%
	PVmax	100%
	Action	Direct
	Mode	Auto
	SP	50%
	Kc	2
	Ti	2

Level Controller Name	**Cond-LC@COL2**	
Tab [Page]	**In this cell...**	**Enter...**
Connections	Process Object	Condenser@ COL2
	Process Variable	Liquid Percent Level
	Output Variable	Reflux
To size the Control Valve for the Reflux stream, select the *Control Valve* button.		
FCV for Reflux	Flow Type	Mass Flow
	Min Available	0.0 lb/hr
	Max Available	5512 lb/hr
Parameters [Configuration]	PVmin	0%
	PVmax	100%
	Action	Direct
	Mode	Auto
	SP	50%
	Kc	1
	Ti	2

Temperature Controllers

Temperature Controller Name	TIC-100	
Tab [Page]	**In this cell...**	**Enter...**
Connections	Process Object	DEA TO PUMP
	Process Variable	Temperature
	Output Variable	COOLER Q
To size the Control Valve for the Cooler Duty stream, select the Control Valve button. To filter high frequency disturbances, click the Parameter tab, select the PV Conditioning page, and change the First Order Time Constant from 15 to 50.		
FCV for COOLER Q	Duty Source	Direct Q
	Min Available	0.0 Btu/hr
	Max Available	2.4e7 Btu/hr
Parameters [Configuration]	PVmin	32 F
	PVmax	122 F
	Action	Direct
	Mode	Auto
	SP	91 F
	Kc	10
	Ti	10
	TIC-103@COL2	
Tab [Page]	**In this cell...**	**Enter...**
Connections	Process Object	Main TS
	Process Variable	Stage Temperature
	Variable Specifics	18_Main TS
	Output Variable	RBLR Q
To size the Control Valve for the Reboiler Duty stream, select the Control Valve button.		
FCV for RBLR Q	Flow Type	Direct Q
	Min Available	0 Btu/hr
	Max Available	1.9e7 Btu/hr
Parameters [Configuration]	PVmin	176 F
	PVmax	302 F
	Action	Reverse
	Mode	Auto
	SP	255°F
	Kc	2
	Ti	5

Pressure Controllers

Pressure Controller Name	PIC-100@COL1	
Tab [Page]	**In this cell...**	**Enter...**

Pressure Controller Name	PIC-100@COL1	
Connections	Process Object	TS-1@COL1
	Process Variable	Top Stage Pressure
	Output Variable	VLV-100@COL1
Parameters [Configuration]	PVmin	950 psia
	PVmax	1050 psia
	Action	Direct
	Mode	Auto
	SP	995 psia
	Kc	2
	Ti	2
	PIC-100@COL2	
Tab [Page]	In this cell...	Enter...
Connections	Process Object	Condenser @COL2
	Process Variable	Vessel Pressure
	Output Variable	VLV-100@COL2
Parameters [Configuration]	PVmin	0 psia
	PVmax	50 psia
	Action	Direct
	Mode	Auto
	SP	31 psia
	Kc	2
	Ti	2

Flow Controller

Flow Controller Name	RECY-FC	
Tab [Page]	In this cell...	Enter...
Connections	Process Object	DEA TO CONT
	Process Variable	Mass Flow
	Output Variable	VLV-103
Parameters [Configuration]	PVmin	0 lb/hr
	PVmax	220460 lb/hr
	Action	Reverse
	Mode	Auto
	SP	97700 lb/hr
	Kc	0.5
	Ti	0.20

G1.6.3 Preparing Dynamic Simulation

Now that the case is ready to run in Dynamic mode, the next step is

installing a strip chart to monitor the general trends of key variables.

Monitoring in Dynamics

You may use several variables in the same chart. If you have a large number of variables that you would like to track, use several Strip Charts rather than use all of the variables on one chart. You may use the same variable in more than one Strip Chart.

For this simulation case, use the Databook (**CTRL D**) to set up two strip charts as defined in the following sections.

StripChart1 - Contactor

Flowsheet	Object	Variable
Case	DEA TO CONT	Mass Flow
Case	GAS TO CONTACTOR	Mass Flow
Case	SWEET GAS	Mass Flow
Case	RICH DEA	Mass Flow
Case	SWEET GAS	Pressure

StripChart2 - Regenerator

Flowsheet	Object	Variable
Case	REGEN FEED	Mass Flow
Case	ACID GAS	Mass Flow
Case	REGEN BTTMS	Mass Flow
Case	ACID GAS	Pressure

1. Start the Integrator and allow the variables to line out.

   If you get an initial numerical error after you start the integrator, start the integrator again. In the Session Preferences view (Simulation tab, Errors group), you can direct these errors to the trace window and have the simulation continue regardless.

   After a few minutes the integrator will stop and an error message will appear in the trace window.
2. From the **Simulation** menu, select **Equation Summary View**.
3. Click the **Uncoverged** tab and click the **Update Sorted List** button.

   The top equation refers to pump P-102. If you examine this pump in the PFD you will see that it is fully on, but its downstream valve has been completely shut by a controller. As an advanced exercise, you

can refine the control scheme to address this issue.

G1.7 References

Gerunda, Arthur. How to Size Liquid-Vapour Separators Chemical Engineering, Vol. 88, No. 9, McGraw-Hill, New York, (1981).

R1 Atmospheric Crude Tower

R1.1 Process Description 2

R1.2 Setup 4

R1.3 Steady State Simulation 7

R1.3.1 Simulate the Pre-Fractionation Train 7
R1.3.2 Install Atmospheric Crude Fractionator 9

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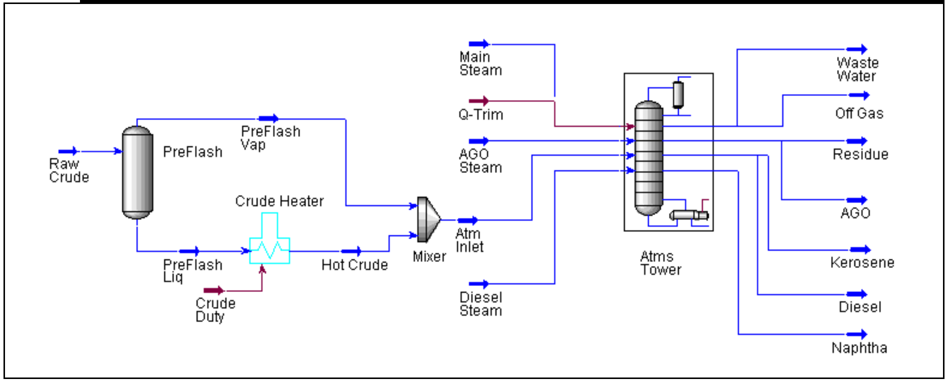
R1.1 Process Description

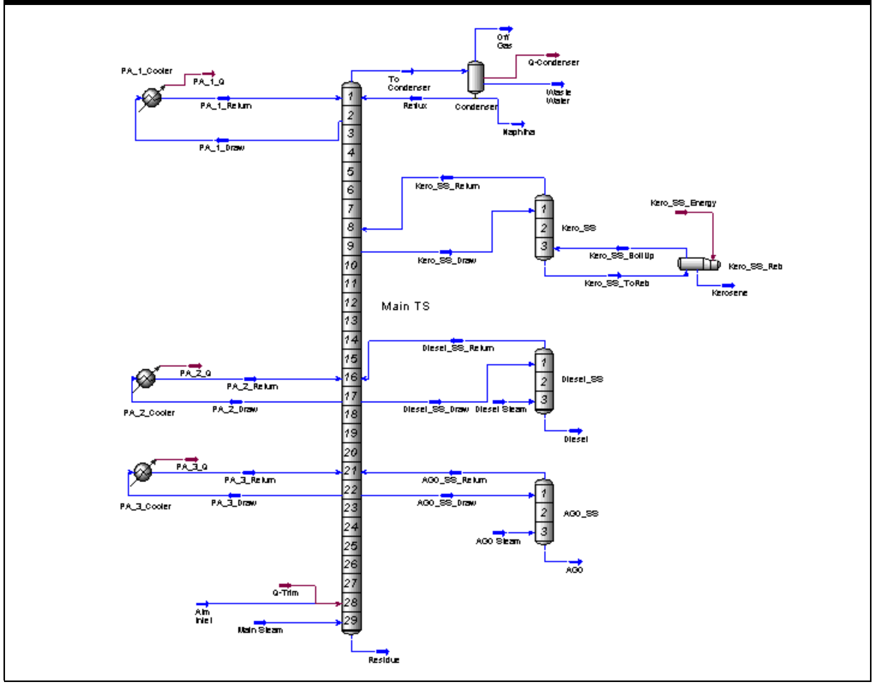
Figure R1.1



After passing through a preheat train, 100,000 barrel/day of 29.32° API crude is fed into a pre-flash separator operating at 450° F and 75 psia. The vapour from this separator bypasses the crude furnace and is re-mixed with the hot (650° F) pre-flash liquids leaving the furnace. The combined stream is then fed to the atmospheric crude column.

The column operates with a total condenser, three coupled side strippers, and three pump around circuits.

Figure R1.2



A naphtha product is produced overhead, a kerosene product is produced from the first side stripper, a diesel product is produced from the second side stripper, and an atmospheric gas oil (AGO) is produced from the third side stripper. Both the AGO side stripper and the diesel side stripper are ‘steam stripped’, while the kerosene side stripper has a reboiler.

The following Assay data is used to characterize the oil for this example:

Assay Liq Volume %	Boiling Temperature (°F)
0.0	15.0
4.5	90.0
9.0	165.0
14.5	240.0
20.0	310.0
30.0	435.0
40.0	524.0
50.0	620.0
60.0	740.0
70.0	885.0
76.0	969.0
80.0	1015.0
85.0	1050.0

Bulk Properties	
Standard Density	29.32° API

Light Ends	Liq Volume %
Methane	0.0065
Ethane	0.0225
Propane	0.3200
i-Butane	0.2400
n-Butane	0.8200
H2O	0.0000

There are two basic steps in this process simulation:

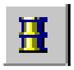
Any other library components required for the overall simulation (e.g., H2O) should be selected as well.

1. **Setup**. The component list must include C1 to C4 light ends components as well as the hypocomponents that will be used to represent the C5+ portion of the crude oil. The Oil Characterization procedure in UniSim Design will be used to convert the laboratory data into petroleum hypocomponents.
2. **Steady State Simulation**. This case will be modeled using a Pre-Fractionation Train consisting of a Separator and Heater. The Outlet stream will then fed to an Atmospheric Crude Fractionator. The results will be displayed.

R1.2 Setup

1. In the Session Preference view, set the unit set to **Field** units.
2. In the Component List view, select the following components: **methane**, **ethane**, **propane**, **i-butane**, **n-butane**, and **water**.
3. In the Fluid Package view, define a fluid package with **Peng-Robinson** as the property package.

Oil Characterization



Oil Environment icon

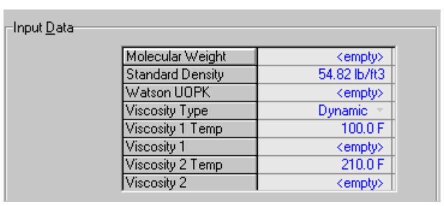
Click the **Oil Environment** icon to enter the Oil Characterization Environment, using the fluid package you just created. Three steps are required for characterizing the oil:

1. Define the Assay.
2. Create the Blend.
3. Install Oil in the Flowsheet.

Define the Assay

1. On the Assay page of the Oil Characterization view, click the **Add** button. This will create a new assay, and you will see the Assay view.
2. Change the **Bulk Properties** setting to **Used**.
3. Complete the Input data for the Bulk Properties as shown below:

Figure R1.3



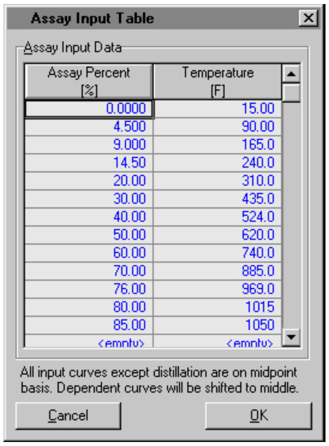
Input Data

Molecular Weight	<empty>
Standard Density	54.82 lb/ft3
Watson UOPK	<empty>
Viscosity Type	Dynamic
Viscosity 1 Temp	100.0 F
Viscosity 1	<empty>
Viscosity 2 Temp	210.0 F
Viscosity 2	<empty>

4. Since the TBP data is supplied, select **TBP** from the Assay Data Type drop-down list.
5. Select **Liquid Volume** from the Assay Basis drop-down list.

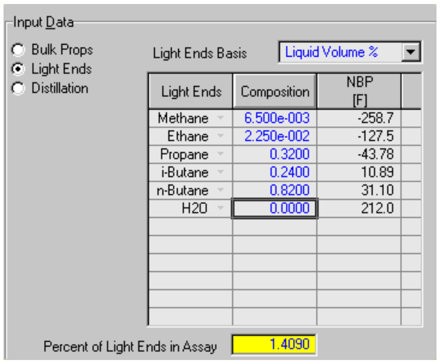
6. Click the **Edit Assay** button and enter the data as indicated in Figure R1.4. When the data entry is complete, click the **OK** button.

Figure R1.4



7. In the Assay Definition group, click the Light Ends drop-down list and select **Input Composition**.
8. In the Input Data group, click the **Light Ends** radio button.
9. Enter the light ends data as follows.

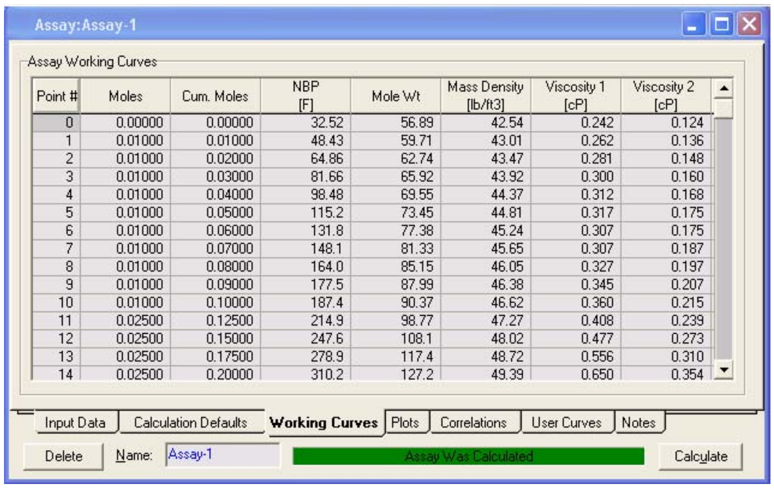
Figure R1.5



You can scroll through this table to view all 50 points of the Working Curve.

10. Upon completion of characterizing the assay, select the **Calculate** button. UniSim Design will calculate the Working Curves, which can be viewed on the **Working Curve** tab.

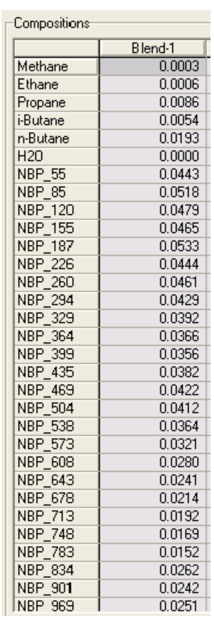
Figure R1.6



Point #	Moles	Cum. Moles	NBP [F]	Mole Wt	Mass Density [lb/ft3]	Viscosity 1 [cP]	Viscosity 2 [cP]
0	0.00000	0.00000	32.52	56.89	42.54	0.242	0.124
1	0.01000	0.01000	48.43	59.71	43.01	0.262	0.136
2	0.01000	0.02000	64.86	62.74	43.47	0.281	0.148
3	0.01000	0.03000	81.66	65.92	43.92	0.300	0.160
4	0.01000	0.04000	98.48	69.55	44.37	0.312	0.168
5	0.01000	0.05000	115.2	73.45	44.81	0.317	0.175
6	0.01000	0.06000	131.8	77.38	45.24	0.307	0.175
7	0.01000	0.07000	148.1	81.33	45.65	0.307	0.187
8	0.01000	0.08000	164.0	85.15	46.05	0.327	0.197
9	0.01000	0.09000	177.5	87.99	46.38	0.345	0.207
10	0.01000	0.10000	187.4	90.37	46.62	0.360	0.215
11	0.02500	0.12500	214.9	98.77	47.27	0.408	0.239
12	0.02500	0.15000	247.6	108.1	48.02	0.477	0.273
13	0.02500	0.17500	278.9	117.4	48.72	0.556	0.310
14	0.02500	0.20000	310.2	127.2	49.39	0.650	0.354

11. Close the Assay view.

Create the Blend (Cut the Oil)



	Blend-1
Methane	0.0003
Ethane	0.0006
Propane	0.0086
i-Butane	0.0054
n-Butane	0.0193
H2O	0.0000
NBP_55	0.0443
NBP_85	0.0518
NBP_120	0.0479
NBP_155	0.0465
NBP_187	0.0533
NBP_226	0.0444
NBP_260	0.0461
NBP_294	0.0429
NBP_329	0.0392
NBP_364	0.0366
NBP_399	0.0356
NBP_435	0.0382
NBP_469	0.0422
NBP_504	0.0412
NBP_538	0.0364
NBP_573	0.0321
NBP_608	0.0280
NBP_643	0.0241
NBP_678	0.0214
NBP_713	0.0192
NBP_748	0.0169
NBP_783	0.0152
NBP_834	0.0262
NBP_901	0.0242
NBP_969	0.0251

1. Click the **Cut/Blend** tab (Oil Characterization view) and click the **Add** button. The Blend: Blend-1 view appears.
2. Click the **Data** tab, then select the Assay you created in the Available Assays column.
3. Click the **Add** button. UniSim Design will transfer that Assay to the Oil Flow Information table.

   As a guideline, each Outlet stream from the crude column should contain a minimum of 5 hypocomponents where the composition is greater than 1.0%. Therefore, a total of 30 components should fulfil this requirement.
4. From the Cut Option Selection drop-down list, select **User Points**, then specify the Number of Cuts at **30**. UniSim Design will calculate the hypocomponents.
5. Click the **Tables** tab to view the hypocomponents.
6. From the Table Type group drop-down list, select **Molar Compositions**.
7. Close the Blend view.

Install Oil in the Flowsheet

The final step is to install the oil in the flowsheet.

1. Click the **Install Oil** tab of the Oil Characterization view.
2. In the Stream Name cell, type **Raw Crude**. This is the stream name where you would like to “install” the oil.
3. On the Oil Characterization view, click **Return to Basis Environment** button.
4. Click the **Enter Simulation Environment** button on the Simulation Basis Manager view to enter the Main Environment. The Raw Crude stream has been installed.

R1.3 Steady State Simulation

The following major steps will be taken to set up this case in steady state:

1. **Simulate the Pre-Fractionation Train**. This determines the feed to the atmospheric fractionator, and includes the pre-flash separation, crude furnace, and mixer which recombines the pre-flash vapour and furnace outlet stream.
2. **Install the Atmospheric Crude Fractionator**. Add the column steam inlets to the flowsheet and install the crude fractionator using the rigorous distillation column operation.

R1.3.1 Simulate the Pre-Fractionation Train

Inlet Stream

Specify the Inlet stream (Raw Crude) as shown below.

Stream [Raw Crude]	
In this cell...	**Enter...**
Temperature [F]	450.0°F
Pressure [psia]	75.0 psia
Std Ideal Liq Vol Flow [barrel/day]	100,000 barrel/day

Because the composition has been transferred from the Oil Characterization, the stream is automatically flashed.

Pre-Flash Operations

Install the Separator, Heater, and Mixer and provide the information displayed below:

Separator [PreFlash]		
Tab [Page]	**In this cell...**	**Enter...**
Design [Connections]	Inlet	Raw Crude
	Vapour Outlet	PreFlash Vap
	Liquid Outlet	PreFlash Liq

Heater [Crude Heater]		
Tab [Page]	**In this cell...**	**Enter...**
Design [Connections]	Inlet	PreFlash Liq
	Outlet	Hot Crude
	Energy	Crude Duty
Design [Parameters]	Delta P	10.00 psi
Worksheet [Conditions]	Temperature (Hot Crude)	650 °F

Mixer [Mixer]		
Tab [Page]	**In this cell...**	**Enter...**
Design [Connections]	Inlets	Hot Crude, PreFlash Vap
	Outlet	Atm Feed

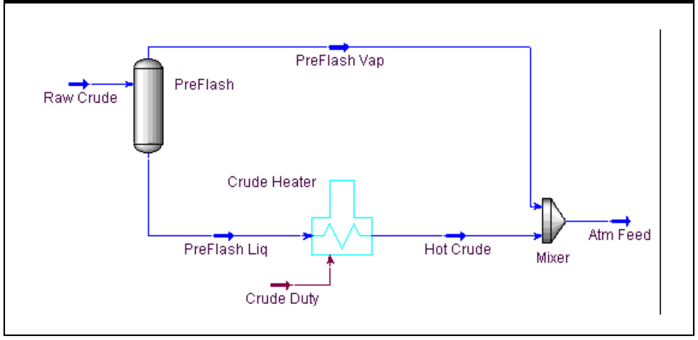
The calculated specifications for the Pre-Fractionation Atm Feed stream appear below.

Figure R1.7

Name	Atm Feed
Vapour Fraction	0.6114
Temperature [F]	622.2
Pressure [psia]	65.00
Molar Flow [lbmole/hr]	6227
Mass Flow [lb/hr]	1.282e+006
Liquid Volume Flow [barrel/day]	1.000e+005
Heat Flow [Btu/hr]	-7.464e+008

The Pre-Fractionation train is shown as follows:

Figure R1.8



R1.3.2 Install Atmospheric Crude Fractionator

Steam and Trim Duty Streams

Before simulating the atmospheric crude tower, the steam feeds and the energy stream (Q-Trim - representing the side exchanger on stage 28) to the column must be defined.

An energy stream can be installed by selecting the appropriate icon from the palette, or by typing into a New Name field on the Energy Streams tab of the Workbook view.

The Q-Trim stream does not require any specifications, this will be calculated by the Column.

These streams could be installed inside the Column Build Environment as well. By taking this approach, you will need to “attach” these streams to the Column Flowsheet so that they can be used in the calculations.

In this application, the **Input Experts** option have been turned off, and the Column is being configured directly through the Property View.

Three steam streams are fed to various locations in the tower. Specify the steam streams as shown below. Define the composition for each as H_2O = **1.0000**.

Stream Name	Temperature [F]	Pressure [psia]	Mass Flow [lb/hr]
Main Steam	375.00	150.00	7500.00
Diesel Steam	300.00	50.00	3000.00
AGO Steam	300.00	50.00	2500.00

Column

The main column, Atms Tower, is represented by the following:

- Number of stages is **29** ideal stages (not including the condenser).
- The overhead condenser operates at **19.7** psia and the bottom stage at **32.7** psia.
- The condenser experiences a **9** psi pressure drop.
- The temperature estimates for the condenser, top stage, and bottom stage are **100**°F, **250**°F and **600**°F, respectively.
- Condensed water is removed via a water draw from the three-phase condenser.

UniSim Design comes with a 3 Stripper Crude Column template. A Refluxed Absorber template could also be used, but this would add the procedure of installing Side Strippers and Pump Arounds.

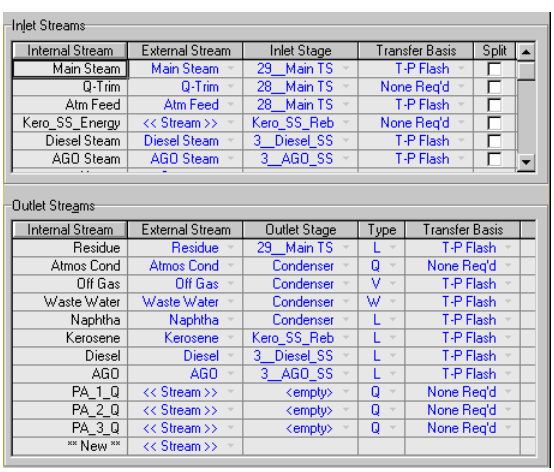
For this example, install the **3 Stripper Crude Column** custom template.

Custom Column icon

1. Select the **Custom Column** icon in the Object Palette, then click the **Read an Existing Column Template** button. The Available Column Templates finder view appears.
2. In the **Files of type** drop-down list, select **Column Templates (*.col)**.
3. From the list, select the **3sscrude.col** template file, then click the **Open** button.

   The 3sscrude.col template installed 40 trays, 29 in the Main Tray section, 3 trays in each of the 3 Side Strippers (1 reboiled and 2 steam stripped), a reboiler, and a condenser.
4. In the Column Property view, connect the Inlet and Outlet streams to the column sub-flowsheet as shown (**Design** tab, **Connections** page).

Figure R1.9


Inlet Streams

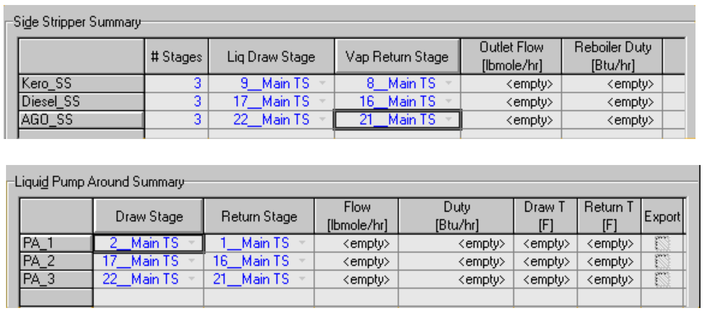
Internal Stream	External Stream	Inlet Stage	Transfer Basis	Split
Main Steam	Main Steam	29__Main TS	T-P Flash	
Q-Trim	Q-Trim	28__Main TS	None Req'd	
Atm Feed	Atm Feed	28__Main TS	T-P Flash	
Kero_SS_Energy	<< Stream >>	Kero_SS_Reb	None Req'd	
Diesel Steam	Diesel Steam	3__Diesel_SS	T-P Flash	
AGO Steam	AGO Steam	3__AGO_SS	T-P Flash	

Outlet Streams

Internal Stream	External Stream	Outlet Stage	Type	Transfer Basis
Residue	Residue	29__Main TS	L	T-P Flash
Atmos Cond	Atmos Cond	Condenser	Q	None Req'd
Off Gas	Off Gas	Condenser	V	T-P Flash
Waste Water	Waste Water	Condenser	W	T-P Flash
Naphtha	Naphtha	Condenser	L	T-P Flash
Kerosene	Kerosene	Kero_SS_Reb	L	T-P Flash
Diesel	Diesel	3__Diesel_SS	L	T-P Flash
AGO	AGO	3__AGO_SS	L	T-P Flash
PA_1_Q	<< Stream >>	<empty>	Q	None Req'd
PA_2_Q	<< Stream >>	<empty>	Q	None Req'd
PA_3_Q	<< Stream >>	<empty>	Q	None Req'd
** New **	<< Stream >>			

5. Modify the Draw and Return stages of the Pump Arounds and Side Strippers on the corresponding page of the **SideOps** tab.

Figure R1.10



Field units are used for column preferences.

6. In the Atmos Tower Column view, specify the column information below.

Column [Atms Tower]		
Tab [Page]	**In this cell...**	**Enter...**
Parameters [Profiles]	Condenser Pressure	19.7 psia
	29_Main TS Pressure	32.7 psia
	Condenser Temperature	100°F
	1_Main TS Temperature	250°F
	29_Main TS Temperature	600°F

Specifications

On the **Monitor** page of the **Design** tab, make the following changes and input the values into the default set of specifications supplied with the pre-built 3-Side Stripper Column.

Open the specification property view by clicking the **View** button, then click **Delete** to delete the specification.

Change the Flow Basis to **Std Ideal Volume** before entering values.

1. Change all the **Pump Around** delta T specifications to a Duty specification.
2. Delete the **Kero SS BoilUp Ratio** and the **Residue Rate** specs.
3. Specify the **Reflux Ratio** spec to have a value of 1. Clear the Reflux Ratio **Active** checkbox and make it an Estimate only.
4. Change the following default specifications by selecting the specification in the table and clicking the **View** button.

Specification	**Flow Basis**	**Spec Type**	**Spec Value**
Kero_SS Prod Flow	Volume		9300 barrel/day
Diesel_SS Prod Flow	Volume		1.925e+04 barrel/day
AGO_SS Prod Flow	Volume		4500 barrel/day
PA_1_Rate(Pa)	Volume		5.000e+04 barrel/day
PA_1_Duty(Pa)		Duty	-5.500e+07 Btu/hr

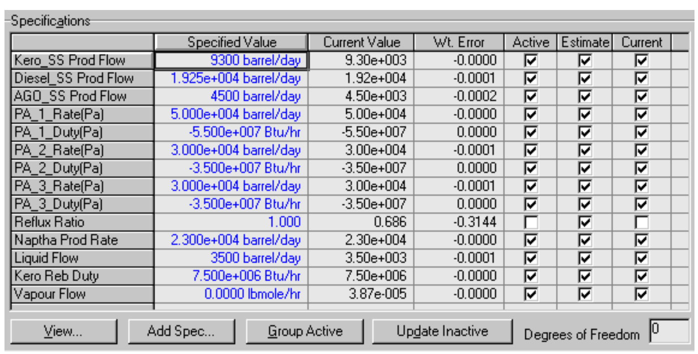
Specification	Flow Basis	Spec Type	Spec Value
PA_2_Rate(Pa)	Volume		3.000e+04 barrel/day
PA_2_Duty(Pa)		Duty	-3.500e+07 Btu/hr
PA_3_Rate(Pa)	Volume		3.000e+04 barrel/day
PA_3_Duty(Pa)		Duty	-3.500e+07 Btu/hr
Naptha Prod Rate	Volume		2.300e+04 barrel/day

5. On the **Specs** page of the **Design** tab, add the following new specifications by clicking the **Add** button in Column Specifications group.

Specification Type	Variable (Field)	Value
Column Liquid Flow	Name	Overflash Spec
	Stages	27_Main TS
	Flow Basis	Std Ideal Vol
	Spec Value	3500.00 barrel/day
Column Duty	Name	Kero Reb Duty
	Energy Stream	Kero_SS_Energy @COL1
	Spec Value	7.5e+6 Btu/hr
Column Vapour Flow	Name	Vap Prod Flow
	Stage	Condenser
	Flow Basis	Molar
	Spec Value	0.00 lbmole/hr

The final specification table will appear as shown below:

Figure R1.11



Specifications

	Specified Value	Current Value	Wt. Error	Active	Estimate	Current
Kero_SS Prod Flow	9300 barrel/day	9.30e+003	-0.0000	☑	☑	☑
Diesel_SS Prod Flow	1.925e+004 barrel/day	1.92e+004	-0.0001	☑	☑	☑
AGO_SS Prod Flow	4500 barrel/day	4.50e+003	-0.0002	☑	☑	☑
PA_1_Rate(Pa)	5.000e+004 barrel/day	5.00e+004	-0.0000	☑	☑	☑
PA_1_Duty(Pa)	-5.500e+007 Btu/hr	-5.50e+007	0.0000	☑	☑	☑
PA_2_Rate(Pa)	3.000e+004 barrel/day	3.00e+004	-0.0001	☑	☑	☑
PA_2_Duty(Pa)	-3.500e+007 Btu/hr	-3.50e+007	0.0000	☑	☑	☑
PA_3_Rate(Pa)	3.000e+004 barrel/day	3.00e+004	-0.0001	☑	☑	☑
PA_3_Duty(Pa)	-3.500e+007 Btu/hr	-3.50e+007	0.0000	☑	☑	☑
Reflux Ratio	1.000	0.686	-0.3144	☐	☑	☐
Naptha Prod Rate	2.300e+004 barrel/day	2.30e+004	-0.0000	☑	☑	☑
Liquid Flow	3500 barrel/day	3.50e+003	-0.0001	☑	☑	☑
Kero Reb Duty	7.500e+006 Btu/hr	7.50e+006	-0.0000	☑	☑	☑
Vapour Flow	0.0000 lbmole/hr	3.87e-005	-0.0000	☑	☑	☑

View... Add Spec... Group Active Update Inactive Degrees of Freedom 0

6. Once you have provided all of the specifications, run the column.

R1.4 Results

Workbook Case (Main)

The material stream results for the Workbook Case[Main] appear below.

Figure R1.12

Workbook - Case (Main)

Name	Raw Crude	PreFlash Vap	PreFlash Liq	Hot Crude	Atm Inlet	AGO Steam
Vapour Fraction	0.2937	1.0000	0.0000	0.4003	0.6122	1.0000
Temperature [F]	450.0	450.0	450.0	650.0	622.2	300.0
Pressure [psia]	75.00	75.00	75.00	65.00	65.00	50.00
Molar Flow [lbmole/hr]	6214	1825	4389	4389	6214	138.8
Mass Flow [lb/hr]	1.282e+006	1.602e+005	1.122e+006	1.122e+006	1.282e+006	2500
Liquid Volume Flow [barrel/day]	1.000e+005	1.490e+004	8.510e+004	8.510e+004	1.000e+005	171.5
Heat Flow [Btu/hr]	-9.192e+008	-1.004e+008	-8.187e+008	-6.447e+008	-7.452e+008	-1.414e+007
Name	Main Steam	Diesel Steam	Residue	Off Gas	Waste Water	Naphtha
Vapour Fraction	1.0000	1.0000	0.0000	1.0000	0.0000	0.0000
Temperature [F]	375.0	300.0	669.1	107.3	107.3	107.3
Pressure [psia]	150.0	50.00	32.70	19.70	19.70	19.70
Molar Flow [lbmole/hr]	416.3	166.5	1397	4.473e-005	700.9	2822
Mass Flow [lb/hr]	7500	3000	6.216e+005	2.304e-003	1.263e+004	2.474e+005
Liquid Volume Flow [barrel/day]	514.6	205.8	4.398e+004	2.612e-004	866.4	2.300e+004
Heat Flow [Btu/hr]	-4.222e+007	-1.697e+007	-3.647e+008	-2.296	-8.561e+007	-2.331e+008
Name	Kerosene	Diesel	AGO	** New **		
Vapour Fraction	0.0000	0.0000	0.0000			
Temperature [F]	457.5	486.8	571.6			
Pressure [psia]	29.84	30.99	31.70			
Molar Flow [lbmole/hr]	701.9	1114	200.4			
Mass Flow [lb/hr]	1.115e+005	2.429e+005	5.945e+004			
Liquid Volume Flow [barrel/day]	9300	1.925e+004	4500			
Heat Flow [Btu/hr]	-8.098e+007	-1.722e+008	-3.882e+007			

Material Streams | Compositions | Energy Streams | Unit Ops

ProductBlock_Kerosene
Atms Tower

Include Sub-Flowsheets
Show Name Only
Number of Hidden Objects: 0

Workbook Case (Atms Tower)

The material stream results for the Workbook Case [Atms Tower]

appear below.

Figure R1.13

Name	Reflux	To Condenser	Main Steam	Residue	4	Off Gas	Water draw
Vapour Fraction	0.0000	1.0000	1.0000	0.0000	0.6122	1.0000	0.0000
Temperature [F]	107.3	274.6	375.0	669.1	622.2	107.3	107.3
Pressure [psia]	19.70	28.70	150.0	32.70	65.00	19.70	19.70
Molar Flow [lbmole/hr]	2010	5532	416.3	1397	6214	4.473e-005	700.9
Mass Flow [lb/hr]	1.763e+005	4.363e+005	7500	6.216e+005	1.282e+006	2.304e-003	1.263e+004
Liquid Volume Flow [barrel/day]	1.638e+004	4.025e+004	514.6	4.398e+004	1.000e+005	2.612e-004	866.4
Heat Flow [Btu/hr]	-1.661e+008	-3.743e+008	-4.222e+007	-3.647e+008	-7.452e+008	-2.296	-8.561e+007

Name	Naphtha	Kero	Kero_SS_Draw	Kero_SS_Retur	Kero_SS_BoilU	Kero_SS_ToRe	Diesel Steam
Vapour Fraction	0.0000	0.0000	0.0000	1.0000	1.0000	0.0000	1.0000
Temperature [F]	107.3	457.5	406.1	429.3	457.5	446.9	300.0
Pressure [psia]	19.70	29.84	29.84	29.84	29.84	29.84	50.00
Molar Flow [lbmole/hr]	2822	701.9	912.4	210.5	371.2	1073	166.5
Mass Flow [lb/hr]	2.474e+005	1.115e+005	1.397e+005	2.816e+004	5.561e+004	1.671e+005	3000
Liquid Volume Flow [barrel/day]	2.300e+004	9300	1.171e+004	2410	4681	1.398e+004	205.8
Heat Flow [Btu/hr]	-2.331e+008	-8.098e+007	-1.063e+008	-1.777e+007	-3.406e+007	-1.225e+008	-1.697e+007

Name	Diesel	Diesel_SS_Dra	Diesel_SS_Ret	AGO	5	AGO_SS_Draw	AGO_SS_Retur
Vapour Fraction	0.0000	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000
Temperature [F]	486.8	512.1	504.9	571.6	300.0	615.4	602.9
Pressure [psia]	30.99	30.99	30.99	31.70	50.00	31.70	31.70
Molar Flow [lbmole/hr]	1114	1331	383.8	200.4	138.8	272.3	210.7
Mass Flow [lb/hr]	2.429e+005	2.800e+005	4.015e+004	5.945e+004	2500	7.563e+004	1.868e+004
Liquid Volume Flow [barrel/day]	1.925e+004	2.231e+004	3269	4500	171.5	5776	1448
Heat Flow [Btu/hr]	-1.722e+008	-1.931e+008	-3.788e+007	-3.882e+007	-1.414e+007	-4.685e+007	-2.217e+007

Name	PA_1_Draw	PA_1_Return	PA_2_Draw	PA_2_Return	PA_3_Draw	PA_3_Return	** New **
Vapour Fraction	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
Temperature [F]	315.9	142.5	512.1	367.4	615.4	485.0	
Pressure [psia]	28.84	28.84	30.99	30.99	31.70	31.70	
Molar Flow [lbmole/hr]	4716	4716	1790	1790	1414	1414	
Mass Flow [lb/hr]	5.740e+005	5.740e+005	3.765e+005	3.765e+005	3.928e+005	3.928e+005	
Liquid Volume Flow [barrel/day]	5.000e+004	5.000e+004	3.000e+004	3.000e+004	3.000e+004	3.000e+004	
Heat Flow [Btu/hr]	-4.697e+008	-5.247e+008	-2.596e+008	-2.946e+008	-2.433e+008	-2.783e+008	

R2 Sour Water Stripper

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R2.3 Steady State Simulation **3**

R2.3.1 Installing the SW Stripper 4

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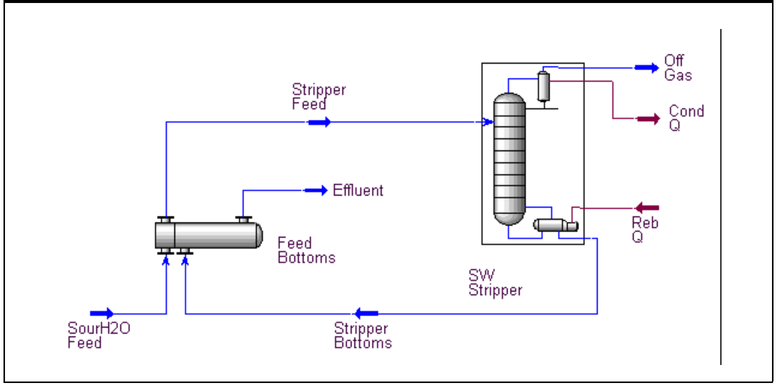
R2.5.1 Results 9

R2.1 Process Description

Figure R2.1

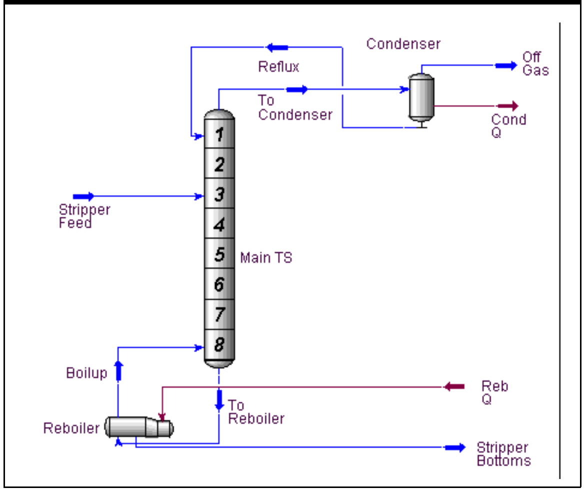


To see this case completely solved, see your UniSim Design\Samples\ directory and open the R-2.usc file.

The sour water stripper configuration shown in the above PFD is a common unit in refineries. It processes sour water that comes from a variety of sources including hydrotreaters, reformers, hydrocrackers, and crude units. The sour water is often stored in crude tanks, thereby eliminating the need for special vapour recovery systems.

A sour water stripper either uses the direct application of stripping steam (usually low quality, low pressure) or a steam-fired reboiler as a heat source.

Figure R2.2



The intent is to drive as much H2S and NH3 overhead in the stripper as possible. The sizing of a sour water stripper is very important since its capacity must equal or exceed the normal production rates of sour water from multiple sources in the refinery. Often, refiners find their strippers undersized due to a lack of allowance for handling large

amounts of sour water, which can result from upset conditions (like start-up and shutdown). Consequently, there is often a backlog of sour water waiting to be processed in the stripper. With the increasing importance of environmental restrictions, the sour water stripper plays a greater role in the overall pollution reduction program of refiners.

The Sour Water feed stream goes through a feed/effluent exchanger where it recovers heat from the tower bottoms stream (Stripper Bottoms). This new stream (Stripper Feed) enters on tray 3 of an 8 tray distillation tower with a reboiler and a total reflux condenser. A quality specification of 10 ppm wt. ammonia on the tower bottoms (Stripper Bottoms) is specified. The tower bottoms, Stripper Bottoms, exchanges heat with the incoming feed and exits as Effluent.

There are two basic steps in this process simulation:

1. **Setup**. This case uses the Sour Peng-Robinson package and the following components: H2S, NH3 and H2O.
2. **Steady State Simulation**. The case will consist of an 8 stage stripper, used to separate H2S and NH3, and a heat exchanger to minimize heat loss.

R2.2 Setup

1. In the Session Preferences view, set the unit set to **Field** units.
2. In the Component List view, select the following components: **H2S**, **NH3** and **H2O**.
3. In the Fluid Package view, select the **Sour PR** property package.

   Sour Peng-Robinson combines the PR equation of state and Wilson's API-Sour model for handling sour water systems.

R2.3 Steady State Simulation

The following general steps will be taken to setup this case in steady state:

1. **Installing the SW Stripper.** An 8 stage distillation column will be used to strip the sour components from the feed stream. The liquid leaving the bottom of the column heats the incoming feed stream in a heat exchanger.
2. **Case Study.** A case study will be performed to obtain steady state solutions for a range of stripper feed temperatures.

R2.3.1 Installing the SW Stripper

Feed Stream

Specify the feed stream as shown below.

Material Stream [SourH2O Feed]	
In this cell...	**Enter...**
Temperature	100°F
Pressure	40 psia
Std Ideal Liq Vol Flow	50,000 barrel/day
Comp Mass Frac [H2S]	0.0070
Comp Mass Frac [NH3]	0.0050
Comp Mass Frac [H2O]	0.9880

Operations

1. Install and specify the Heat Exchanger as shown below.

Heat Exchanger [Feed Bottoms]		
Tab[Page]	**In this cell...**	**Enter...**
Design [Connections]	Tube Side Inlet	Sour H2O Feed
	Tube Side Outlet	Stripper Feed
	Shell Side Inlet	Stripper Bottoms
	Shell Side Outlet	Effluent
Design [Parameters]	Heat Exchanger Model	Exchanger Design (Weighted)
	Tube Side Delta P	10 psi
	Shell Side Delta P	10 psi
Worksheet [Conditions]	Temperature (Stripper Feed)	200°F

2. Install a Distillation Column. This column will have both a reboiler and an overhead condenser.

If messages appear regarding loading an older case or installing property sets, click the **OK** button. They will not affect the case.

3. Define the Column configuration as shown below.

Column [SW Stripper]		
Page	**In this cell...**	**Enter...**
Connections	No. of Stages	8
	Inlet Stream	Stripper Feed
	Inlet Stage	3
	Condenser Type	Full Reflux
	Ovhd Vapour	Off Gas
	Bottoms Liquid	Stripper Bottoms
	Reboiler Energy Stream	Q-Reb
	Condenser Energy Steam	Q-Cond
Pressure Profile	Condenser Pressure	28.7 psia
	Reboiler Pressure	32.7 psia

4. In the Column property view, click the **Design** tab, then select the **Monitor** page.

   In the present configuration, the column has two degrees of freedom. For this example, the two specifications used will be a quality specification and a reflux ratio.

5. Modify the existing specification based on the information below:

Column [SW Stripper]		
Tab [Page]	**Variable Spec**	**Modify**
Design [Specs]	Ovhd Vap Rate	Active = uncheck
	Reflux Ratio	Active = checked Spec Value = 10 Molar

To add a new specification, click the **Add Spec** button.

6. Add a **Component Fraction** specification, and enter the following information in the **Comp Frac Spec** view:

Tab	In this cell...	Enter...
Parameters	Name	NH3 Mass Frac (Reboiler)
	Stage	Reboiler
	Spec Value	0.000010
	Component	Ammonia
Summary	Active	Checked
	Reflux Ratio Spec Value	Active 10 Molar

For more information on which damping factor is recommended for different systems, refer to **Chapter 8 - Column** of the **UniSim Design Operations Guide**.

7. Click the **Parameters** tab, then select the **Solver** page. Change the Fixed Damping Factor to **0.4**.

   A damping factor will speed up tower convergence and reduce the effects of any oscillations in the calculations (the default value is 1.0).

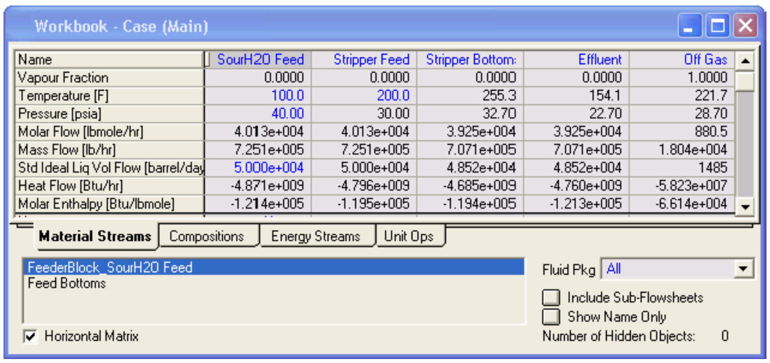
8. Run the column to calculate the values by clicking the **Run** button.

R2.4 Results

Workbook Case (Main)

Materials Streams Tab

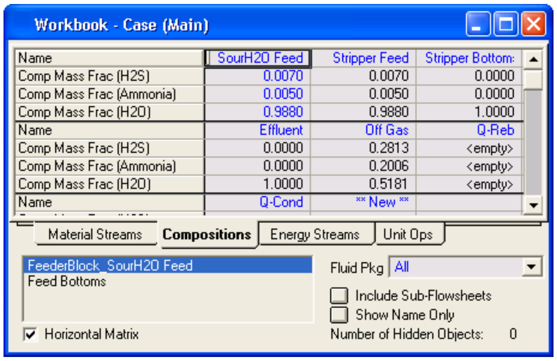
Figure R2.3



Name	SourH2O Feed	Stripper Feed	Stripper Bottom:	Effluent	Off Gas
Vapour Fraction	0.0000	0.0000	0.0000	0.0000	1.0000
Temperature [F]	100.0	200.0	255.3	154.1	221.7
Pressure [psia]	40.00	30.00	32.70	22.70	28.70
Molar Flow [lbmole/hr]	4.013e+004	4.013e+004	3.925e+004	3.925e+004	880.5
Mass Flow [lb/hr]	7.251e+005	7.251e+005	7.071e+005	7.071e+005	1.804e+004
Std Ideal Liq Vol Flow [barrel/day	5.000e+004	5.000e+004	4.852e+004	4.852e+004	1485
Heat Flow [Btu/hr]	-4.871e+009	-4.796e+009	-4.685e+009	-4.760e+009	-5.823e+007
Molar Enthalpy [Btu/lbmole]	-1.214e+005	-1.195e+005	-1.194e+005	-1.213e+005	-6.614e+004

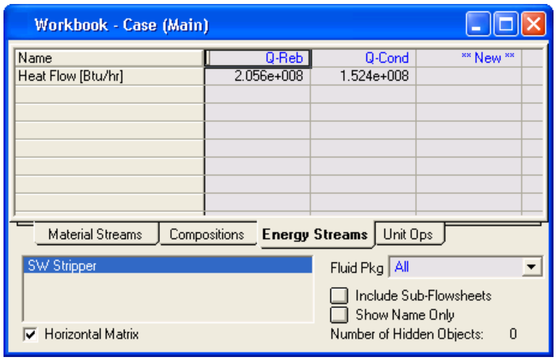
Compositions Tab

Figure R2.4



Energy Streams Tab

Figure R2.5



R2.5 Case Study

The simulation can be run for a range of Stripper Feed temperatures (e.g., 190°F through 210°F in 5 degree increments) by changing the temperature specified for Stripper Feed in the worksheet.

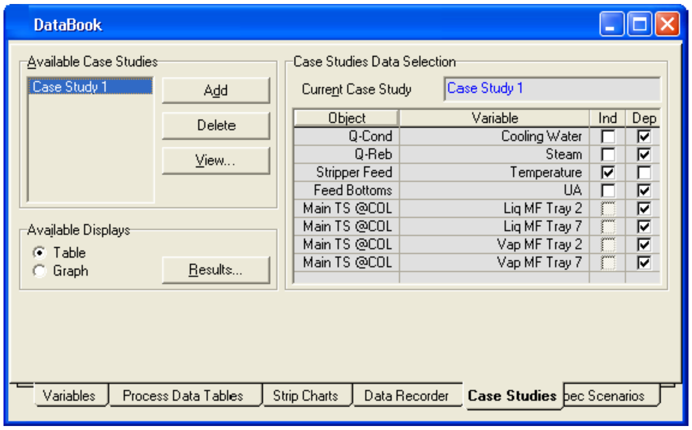
You can automate these changes by using the Case Studies feature in the DataBook.

1. Open the DataBook property view (Tools menu).
2. On the **Variables** tab, enter the variables as shown below.

Flowsheet	Object	Variables	Variables Description
Case	Q-Cond	Heat Flow	Cooling Water
	Q-Reb	Heat Flow	Steam
	Stripper Feed	Temperature	Temperature
	Feed Bottoms	UA	UA
T-100 SW Stripper	Main TS	Stage Liq Net Mass Flow (2__Main TS)	Liq MF Tray 2
	Main TS	Stage Liq Net Mass Flow (7__Main TS)	Liq MF Tray 7
	Main TS	Stage Vap Net Mass Flow (2__Main TS)	Vap MF Tray 2
	Main TS	Stage Vap Net Mass Flow (7__Main TS)	Vap MF Tray 7

3. Click the **Case Studies** tab.
4. In the Available Case Studies group, click the **Add** button to create Case Study 1.
5. Check the Independent and Dependent Variables as shown below.

Figure R2.6

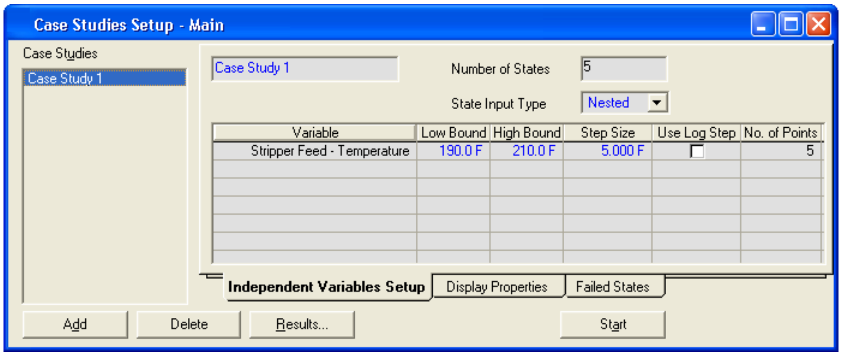


To automate the study, the Independent Variable range and Step Size must be given.

Temperature values are given in °F.

6. Click the **View** button to access the Case Studies Setup view. Define the range and step size for the Stripper Feed Temperature as shown below.

Figure R2.7

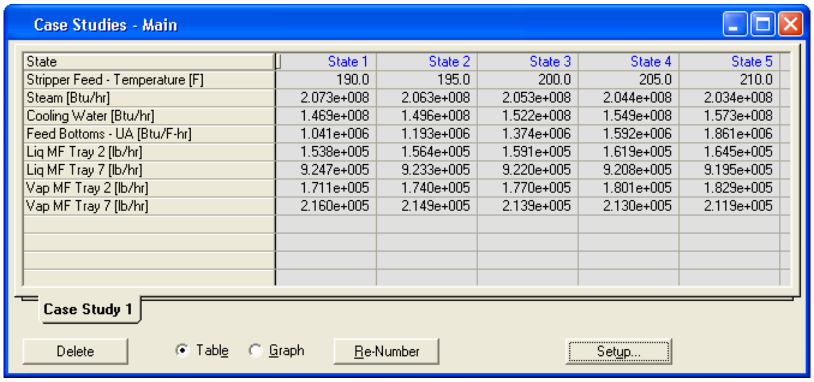


7. To begin the Study, click the **Start** button.
8. Click the **Results** button to view the variables. If the results are in graphical form, click the **Table** radio button on the Case Studies view.

R2.5.1 Results

The results of this study appear below.

Figure R2.8



State	State 1	State 2	State 3	State 4	State 5
Stripper Feed - Temperature [F]	190.0	195.0	200.0	205.0	210.0
Steam [Btu/hr]	2.073e+008	2.063e+008	2.053e+008	2.044e+008	2.034e+008
Cooling Water [Btu/hr]	1.469e+008	1.496e+008	1.522e+008	1.549e+008	1.573e+008
Feed Bottoms - UA [Btu/F-hr]	1.041e+006	1.193e+006	1.374e+006	1.592e+006	1.861e+006
Liq MF Tray 2 [lb/hr]	1.538e+005	1.564e+005	1.591e+005	1.619e+005	1.645e+005
Liq MF Tray 7 [lb/hr]	9.247e+005	9.233e+005	9.220e+005	9.208e+005	9.195e+005
Vap MF Tray 2 [lb/hr]	1.711e+005	1.740e+005	1.770e+005	1.801e+005	1.829e+005
Vap MF Tray 7 [lb/hr]	2.160e+005	2.149e+005	2.139e+005	2.130e+005	2.119e+005

P1 Propylene/Propane Splitter

P1.1 Process Description **2**

P1.2 Setup **3**

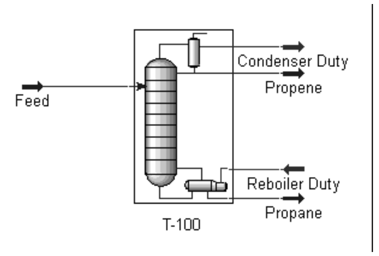
P1.3 Steady State Simulation **3**

P1.3.1 Starting the Simulation 3
P1.3.2 Adding the Stripper (Reboiled Absorber) 4
P1.3.3 Adding the Rectifier (Refluxed Absorber) 5
P1.3.4 Adding the Specifications 6

P1.4 Results **7**

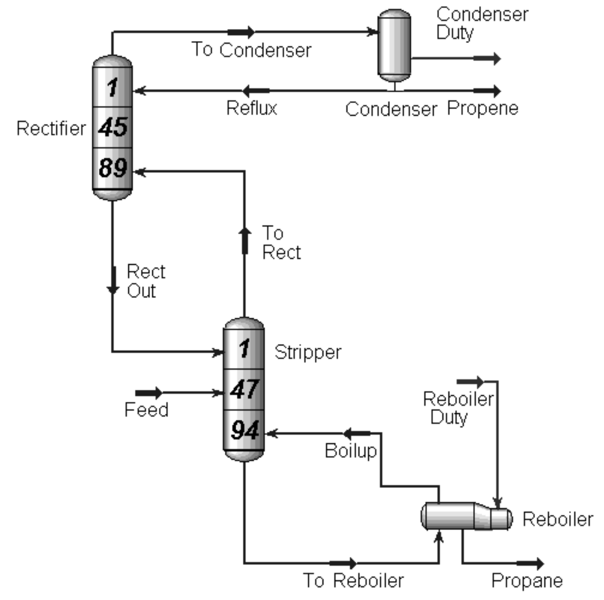
P1.1 Process Description

Figure P1.1



A propylene-propane splitter is generally an easy column to converge. The critical factor in producing good results, however, is not the ease of solution, but the accurate prediction of the relative volatility of the two key components. Special consideration was given to these components, and others, in developing the binary interaction coefficients for the Peng Robinson and Soave Redlich Kwong Equations of State to ensure that these methods correctly model this system.

Figure P1.2



These splitters have many stages and are often built as two separate columns. This simulation will contain two Columns, a Stripper, and a Rectifier. The Stripper is modeled as a Reboiled Absorber and contains 94 theoretical stages. The Rectifier is a Refluxed Absorber containing 89 theoretical stages. The Stripper contains two feed streams, one is the

known stream, FEED, and the other is the bottoms from the Rectifier. Propane is recovered from the Stripper bottoms (95%) and Propene is taken off the top of the Rectifier (99%).

There are two basic steps in this process simulation:

1. Setup. The Soave Redlich Kwong (SRK) property package will be used and the component list includes Propane and Propene.
2. Steady State Simulation. The case will consist of a column divided into two tray sections: a Refluxed Absorber as a Rectifier and a Reboiled Absorber as a Stripper.

P1.2 Setup

1. In the Session Preferences view, set the unit set to Field units.
2. In the Component List view, select the following two components: Propane and Propene.

   It may be easier to search by chemical formula (C3H8 and C3H6), as the entire list is quite extensive.
3. In the Fluid Package view, select the Soave Redlich Kwong (SRK) equation of state (EOS) as the property method for this case.

   Ensure that the selected component you just created appears in the Component List Selection drop-down list.

P1.3 Steady State Simulation

The case will be setup in steady state using the Custom Column option. Both the Rectifier and Stripper columns will be built in the same column environment.

P1.3.1 Starting the Simulation

Defining the Feed Stream

In the Main Simulation environment, define the conditions and compositions of the Feed stream as shown in the following table.

Material Stream [Feed]	
In this cell...	**Enter...**
Name	Feed
Vapour Frac	1.0
Pressure	300 psia
Molar Flow	1350 lbmole/hr

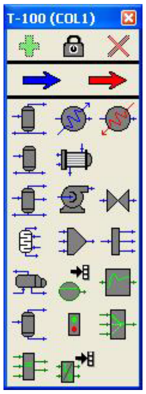
Material Stream [Feed]	
Comp Mole Frac [Propane]	0.4
Comp Mole Frac [Propene]	0.6

Installing the Column

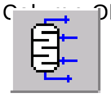
1. Click the Custom Column icon on the Object Palette. The Custom Column feature will be used to build both columns in a single column environment.
2. Click the Start with a Blank Flowsheeet button. The column appears in the PFD.
3. Double-click the column in the PFD to open the Column view.
4. Click the Design tab and select the Connections page.
5. In the Inlet Streams group, enter stream Feed as an External Feed Stream, making this stream accessible to the Template Environment.
6. Enter the Column Environment by clicking the Column Environment button at the bottom of the Column property view.

For this example, you will need a Total Condenser, Reboiler and two Tray Sections. A Tray Section and a Condenser will be used for the Refluxed Absorber (Rectifier), a Reboiler and another Tray Section will be used for the Reboiled Absorber (Stripper). The overhead product from the Stripper will serve as the feed to the Rectifier, and the bottoms product from the Rectifier provides a second feed to the Stripper, entering at Stage 1.

P1.3.2 Adding the Stripper (Reboiled Absorber)



Column Object Palette


Tray Section icon

Install the Reboiled Absorber before the Reboiler. This column has 94 ideal stages and a Reboiler.

Ensure that you are within the Column Environment; the PFD view and the Column Object Palette should be visible (as shown on the left).

Installing the Tray Section

For this Column a new Tray Section has to be installed.

1. Double-click the Tray Section icon on the Column Object Palette. The tray section appears in the PFD and the Tray Section property

view appears.

2. Supply the following information.

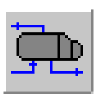
Tray Section [Stripper]		
Tab [Page]	**In this cell...**	**Enter...**
Design [Connections]	Column Name	Stripper
	Liquid Inlet	Rect Out
	Vapour Inlet	Boilup
	Vapour Outlet	To Rect
	Liquid Outlet	To Reboiler
	Optional Feed Streams	Feed (Stage 47)
Design [Parameters]	Number of Trays	94
Design [Pressures]	Tray 1	290 psia
	Tray 94	300 psia

Define the Number of Trays on the Parameters page first.

3. Close the Tray Section view.

Installing the Reboiler

The Reboiler for the Absorber must be installed with the Stripper Column.



Reboiler icon

1. Double-click the Reboiler icon on the Column Object Palette. The Reboiler appears in the PFD and the Reboiler property view appears.
2. Enter the following information.

Reboiler [Reboiler]		
Tab [Page]	**In this cell...**	**Enter...**
Design [Connections]	Name	Reboiler
	Boilup	Boilup
	Inlets	To Reboiler
	Bottoms Outlet	Propane
	Energy	Reboiler Duty

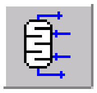
P1.3.3 Adding the Rectifier (Refluxed Absorber)

Next, you will install the Rectifier. This column has 89 ideal stages and a Total Condenser.

Installing the Tray Section

Install a new Tray Section for the Absorber.

1. Double-click the Tray Section icon on the Object Palette.
2. In the Tray Section view, supply the parameters as shown below.



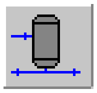
Tray Section icon

Tray Section [Rectifier]		
Tab [Page]	**In this cell...**	**Enter...**
Design [Connections]	Name	Rectifier
	Liquid Inlet	Reflux
	Vapour Inlet	To Rect
	Vapour Outlet	To Condenser
	Liquid Outlet	Rect Out
Design [Parameters]	Number of Trays	89
Design [Pressures]	Tray 1	280 psia
	Tray 89	290 psia

3. Close the Tray Section view.

Installing the Total Condenser

A Total Condenser is required for the column.



Total Condenser icon

1. Double-click the Total Condenser icon in the Object Palette. The condenser icon appears in the PFD, and the condenser property view appears.
2. Supply the following information.

Total Condenser [Condenser]		
Tab [Page]	**In this cell...**	**Enter...**
Design [Connections]	Name	Condenser
	Inlets	To Condenser
	Distillate	Propene
	Reflux	Reflux
	Energy	Condenser Duty

P1.3.4 Adding the Specifications

Two specifications are required for this column.

- Flow of the Rectifier Distillate (Propene) is 775 lbmole/hr.
- Rectifier Top Stage Reflux Ratio is 16.

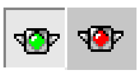
1. Return to the Parent environment and ensure the Column property view is visible.
2. Click the Design tab and select Monitor page.
3. Add a Column Draw Rate and Column Reflux Ratio specifications.

To add a specification, click the Add Spec button.

4. Enter the following information for the appropriate specification:

Column Draw Rate		
Tab	**In this cell...**	**Enter...**
Parameters	Draw	Propene
	Flow Basis	Molar
	Spec Value	775 lbmole/hr.

Column Reflux Ratio		
Tab	**In this cell...**	**Enter...**
Parameter	Stage	Condenser
	Flow Basis	Molar
	Spec Value	16.4



Run Column Solver icon (green)

Hold Column Solver icon (red)

If the column has not converged at this point, ensure the Run Column Solver icon is active.

P1.4 Results

Go to the Workbook of the Column:T-100 column environment to check the following results.

Material Streams Tab

Figure P1.3

Workbook - T-100 (COL1)

Name	Feed	Rect Out	Boilup	To Rect	To Reboiler
Vapour Fraction	1.0000	0.0000	1.0000	1.0000	0.0000
Temperature [F]	126.7	121.1	135.1	121.1	135.0
Pressure [psia]	300.0	290.0	300.0	290.0	300.0
Molar Flow [lbmole/hr]	1350	1.294e+004	1.284e+004	1.372e+004	1.341e+004
Mass Flow [lb/hr]	5.790e+004	5.502e+005	5.639e+005	5.828e+005	5.892e+005
Liquid Volume Flow [barrel/day]	7698	7.276e+004	7.604e+004	7.705e+004	7.945e+004
Heat Flow [Btu/hr]	-1.729e+007	-1.048e+008	-5.158e+008	-3.209e+007	-6.060e+008
Name	Propane	Reflux	To Condenser	Propene	** New **
Vapour Fraction	0.0000	0.0000	1.0000	0.0000	
Temperature [F]	135.1	116.0	116.0	116.0	
Pressure [psia]	300.0	280.0	280.0	280.0	
Molar Flow [lbmole/hr]	574.9	1.271e+004	1.349e+004	775.1	
Mass Flow [lb/hr]	2.527e+004	5.352e+005	5.678e+005	3.263e+004	
Liquid Volume Flow [barrel/day]	3408	7.036e+004	7.465e+004	4290	
Heat Flow [Btu/hr]	-2.626e+007	3.350e+007	1.064e+008	2.043e+006	

Material Streams | Compositions | Energy Streams | Unit Ops

Feed @Main
Stripper

Show Name Only
Number of Hidden Objects: 0

Compositions Tab

Figure P1.4

Workbook - T-100 (COL1)

Name	Feed	Rect Out	Boilup	To Rect	To Reboiler
Comp Mole Frac (Workbook) (Pr	0.4000	0.2145	0.9153	0.2029	0.9157
Comp Mole Frac (Workbook) (Pr	0.6000	0.7855	0.0847	0.7971	0.0843
Name	Propane	Reflux	To Condenser	Propene	** New **
Comp Mole Frac (Workbook) (Pr	0.9251	0.0105	0.0105	0.0105	
Comp Mole Frac (Workbook) (Pr	0.0749	0.9895	0.9895	0.9895	

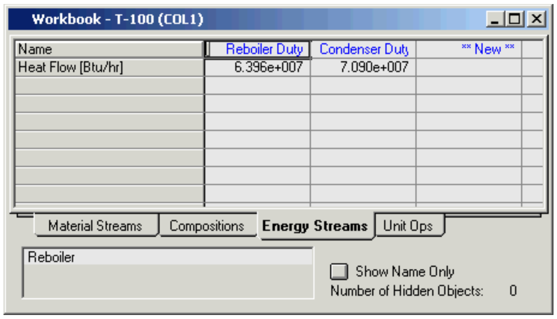
Material Streams | **Compositions** | Energy Streams | Unit Ops

Feed @Main
Stripper

Show Name Only
Number of Hidden Objects: 0

Energy Streams Tab

Figure P1.5



C1 Ethanol Plant

C1.1 Process Description 2

C1.2 Setup 4

C1.3 Steady State Simulation 5

C1.3.1 Adding Streams 5
C1.3.2 Installing Equipment 5
C1.3.3 Draw Stream Location 10

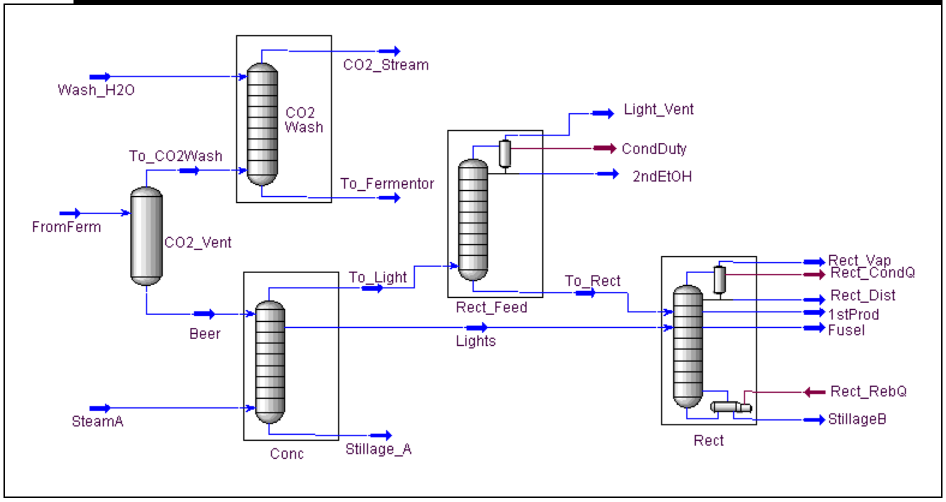
C1.4 Results 12

C1.1 Process Description

Typically, an ethanol fermentation process produces mainly Ethanol plus small quantities of several by-products: methanol, 1-propanol, 2-propanol, 1-butanol, 3-methyl-1-butanol, 2-pentanol, acetic acid, and CO2.

To see this case completely solved, see your UniSim Design\Samples\ directory and open the **C-2.usc** file.

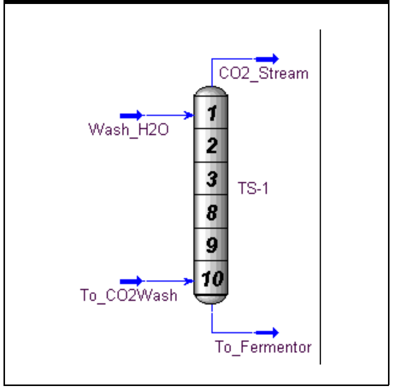
Figure C1.1



Ethanol and Water form an azeotropic mixture at 1 atm. Therefore, with simple distillation, the ethanol and water mixture can only be concentrated up to the azeotropic concentration.

The CO2 produced in the fermentation vessel carries some ethanol. This CO2 stream is washed with water in a vessel (CO2 Wash) to recover the Ethanol, which is recycled to the fermentor.

Figure C1.2

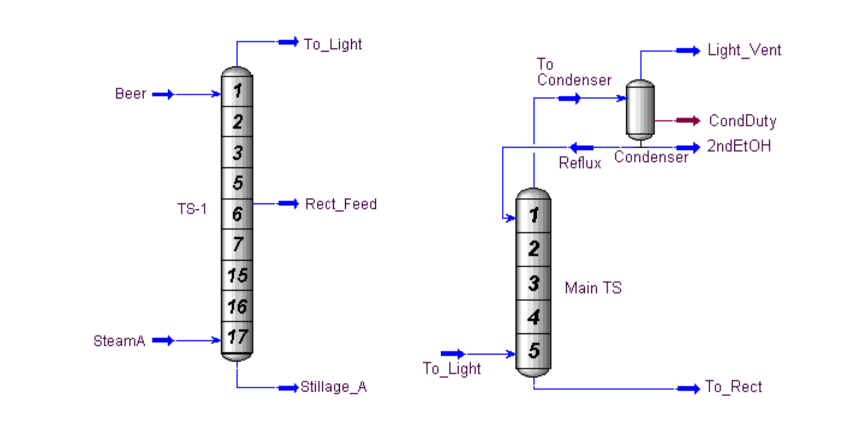


The Ethanol rich product stream from the fermentor is sent to a concentration (Conc) tower. An absorber with a side vapour draw can be

used to represent this tower.

The top vapour is fed to a light purification tower (Lights) where most of the remaining CO2 and some light alcohols are vented. The bottom product of this light tower is fed to the Rectifier.

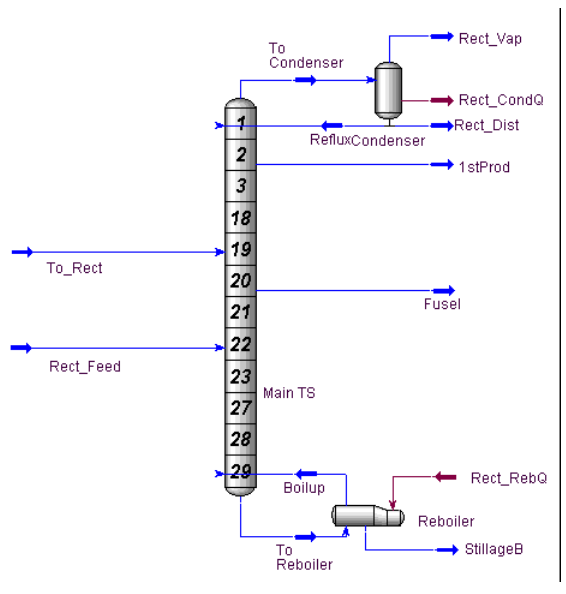
Figure C1.3



The side vapour draw from the Concentrator is the main feed for the Rectifier. The Rectifier is operated as a conventional distillation tower. The product of this tower is taken from Stage 2 so to have an azeotropic ethanol product with a lesser methanol contamination. Methanol concentrates towards the top stages, so a small distillate draw is provided at the condenser. Also, a small vent for CO2 is

provided at the condenser.

Figure C1.4



Fusel oils are a mixture of propanols, butanols, and pentanols that have a potential value superior to that of ethanol. Accumulation of fusel oils in the Rectification Tower can cause the formation of a second liquid phase and subsequent deterioration of performance for these trays, so small side liquid draws of fusel oils are installed on the rectifier to avoid this problem.

Another factor of interest is the concentration of heavy alcohols in the interior of the Rectifier. These alcohols are normally referred to as Fusel oils, and a small side liquid draw is provided in the Rectifier to recover these components.

There are two general steps in this process simulation:

1. **Setup**. The NRTL property package and the UNIFAC VLE estimation method will be used for this case. The Components list includes Ethanol, H2O, CO2, Methanol, Acetic Acid, 1- Propanol, 2-Propanol, 1-Butanol, 3-M-1-C4ol, 2-Pentanol and Glycerol.
2. **Steady State Simulation**. This case will use a separator, two absorbers, a refluxed absorber and a distillation column.

C1.2 Setup

1. In the Session Preferences view, set the unit set to **SI**.
2. In the Component List view, select the following components: **Ethanol**, **H2O**, **CO2**, **Methanol**, **Acetic Acid**, **1-Propanol**, **2-Propanol**, **1-Butanol**, **3-M-1-C4ol**, **2-Pentanol**, and **Glycerol**.
3. In the Fluid Package view, select **NRTL** as the property package.
4. On the **Binary Coeffs** tab of the Fluid Package view, select the **UNIFAC VLE** radio button and click the **Unknowns Only** button to estimate the missing interaction parameters.

C1.3 Steady State Simulation

C1.3.1 Adding Streams

Once you have entered the Mole Fractions for the stream FromFerm, the Mole Fractions will not add up to 1.00. Click the **Normalize** button and the total Mole Fraction will equal 1.00.

Enter the Simulation environment and add the material streams defined below.

Name	Wash H2O	FromFerm	Steam A
In this cell...	**Enter...**	**Enter...**	**Enter...**
Temperature [C]	25	30	140
Pressure [kPa]	101.3250	101.3250	101.3250
Molar Flow [kgmole/hr]	130	2400	
Mass Flow [kg/hr]			11000
Comp Mole Frac [Ethanol]	0.0000	0.0269	0.0000
Comp Mole Frac [H2O]	1.0000	0.9464	1.0000
Comp Mole Frac [CO2]	0.0000	0.0266	0.0000
Comp Mole Frac [Methanol]	0.0000	2.693e-05	0.0000
Comp Mole Frac [Acetic Acid]	0.0000	3.326e-06	0.0000
Comp Mole Frac [1-Propanol]	0.0000	9.077e-06	0.0000
Comp Mole Frac [2-Propanol]	0.0000	9.096e-06	0.0000
Comp Mole Frac [1-Butanol]	0.0000	6.578e-06	0.0000
Comp Mole Frac [3-M-1-C4ol]	0.0000	2.148e-05	0.0000
Comp Mole Frac [2-Pentanol]	0.0000	5.426e-06	0.0000
Comp Mole Frac [Glycerol]	0.0000	6.64e-06	0.0000

C1.3.2 Installing Equipment

CO2 Vent Separator

The CO2Vent Separator separates the products from the fermentor. The bottom liquid of the separator is sent to the distillation section of the plant (Concentrator Tower), while the overhead vapour goes to the CO2Wash Tower.

Install a Separator and make the connections shown below.

SEPARATOR [CO2 Vent]		
Tab [Page]	**In this cell...**	**Enter...**
Design [Connections]	Inlets	FromFerm
	Vapour Outlet	To CO2Wash
	Liquid Outlet	Beer

CO2 Wash Tower

Water is used to strip any Ethanol entrained in the off gas mixture, thus producing an overhead of essentially pure CO2. The bottom product from the tower is recycled to the Fermentor, however, the recycle is not a concern in this example.

1. Before installing the column, select **Preferences** from the UniSim Design Tools menu.
2. On the **Options** page of the **Simulation** tab, ensure that the **Use Input Experts** checkbox is checked, then close the view.
3. Install the CO2 Wash Tower as a simple Absorber.

Absorber [CO2WASH]		
Tab [Page]	**In this cell...**	**Enter...**
Connections	No. of Stages	10
	Top Stage Inlet	Wash H2O
	Bottom Stage Inlet	To CO2Wash
	Ovhd Vapour	CO2 Stream
	Bottoms Liquid	To fermentor
Pressure Profile	Top Stage	101.325 kPa
	Bottom Stage	101.325 kPa

4. Click the **Run** button in the Column property view to calculate the CO2 Wash Tower product streams.

Concentrator

1. Install the Concentrator as an Absorber with a side vapour draw.

Absorber [CONC]		
Tab [Page]	**In this cell...**	**Enter...**
Connections	No. of Stages	17
	Top Stage Inlet	Beer
	Bottom Stage Inlet	Steam A
	Ovhd Vapour	To Light
	Bottoms Liquid	Stillage A
	Side Draw Vapour	Rect Feed (Stage 6)
Pressure Profile	Top Stage	101.325 kPa
	Bottom Stage	102.325 kPa
Temperature Estimates	Condenser Temperature	90°C
	Reboiler Temperature	110°C

You might have to deactivate the default Rect Feed Rate specification to converge the column.

2. Create and define the following specifications to fully specify the column.

Specifications		
Tab [Page]	**In this cell...**	**Enter...**
Design [Specs]	Comp Recovery Draw SpecValue Component	Active Rect Feed 0.95 Ethanol
	Draw Rate 1 Draw Flow Basis Spec Value	Estimate Rect Feed Mass 5000 kg/h
	Draw Rate 2 Draw Flow Basis Spec Value	Estimate To_Light Molar 1000 kgmole/h

3. Click the **Run** button in the Column property view to calculate the Concentrator product streams.

Lights

1. Add the Lights Tower purification tower, modeled as a Refluxed Absorber, and define as indicated below.

Refluxed Absorber [Lights]		
Tab [Page]	**In this cell...**	**Enter...**
Connections	No. of Stages	5
	Bottom Inlet Streams	To Light
	Condenser Type	Partial
	Ovhd Vapour	Light Vent
	Ovhd Liquid	2ndEtOH
	Bottoms Liquid	To Rect
	Cond. Energy	CondDuty
Pressure Profile	Condenser	101.325 kPa
	Bottom Stage	101.325 kPa

2. Delete the default **Btms Prod Rate** and **Reflux Rate** specifications from the Column Specification group.

3. Add the following new column specifications (**Design** tab, **Specs** page).

Specifications		
Tab [Page]	**In this cell...**	**Enter...**
Design [Specs]	Vap Prod Rate Draw Flow Basis Spec Value	Active Light_Vent Molar 1.6 kgmole/hr
	Comp Fraction Stage Flow Basis Phase Spec Value Component	Active Condenser Mass Fraction Liquid 0.88 Ethanol
	Reflux Ratio Stage Flow Basis Spec Value	Estimate Condenser Molar 5.00
	Distillate Rate Draw Flow Basis Spec Value	Estimate 2ndEtOH Molar 2.10 kgmole/hr

4. If required, click the **Run** button in the Column property view to calculate the Light Tower product streams.

Rectifier

The primary product from a plant such as this would be the azeotropic mixture of ethanol and water. The Rectifier serves to concentrate the water/ethanol mixture to near azeotropic composition. The Rectifier is operated as a conventional distillation tower. It contains a partial condenser as well as a reboiler.

1. Add the Rectifier column, modeled as a distillation tower, and define

it using the following information.

Column [RECT]		
Tab [Page]	**In this cell...**	**Enter...**
Connections	No. of Stages	29
	Inlet Streams [Stage]	To Rect [19], Rect_Feed [22]
	Condenser Type	Partial
	Ovhd Vapour	Rect Vap
	Ovhd Liquid	Rect Dist
	Bottoms Liquid	Stillage B
	Reboiler Energy	Rect RebQ
	Condenser Energy	Rect CondQ
	Side Draw Liquid [Stage]	1st Prod [2], Fusel [20]
Pressure Profile	Condenser Pressure	101.325 kPa
	Reboiler Pressure	101.325 kPa
Temperature Estimates	Condenser	79°C
	Reboiler	100°C

2. Delete the default **Btms Prod Rate** and **Reflux Rate** specifications before adding the new specifications. Delete all specifications that do not appear in the following table.

3. Define the following specifications (**Design** tab, **Specs** page). Also, set the damping factor to accelerate the convergence.

Specifications		
Tab [Page]	**In this cell...**	**Enter...**
Design [Specs]	Reflux Ratio Stage Flow Basis Spec Value	Active Condenser Molar 7100
	Ovhd Vap Rate Draw Flow Basis Spec Value	Active Rect_Vap Molar 0.100 kgmole/hr
	Draw Rate Draw Flow Basis Spec Value	Active Rect _Dist Mass 2.00 kg/hr
	Comp Frac Stage Flow Basis Phase Spec Value Component	Active 2_Main TS Mass Fraction Liquid 0.95 Ethanol
	Fusel Draw Rate Draw Flow Basis Spec Value	Active Fusel Mass 3.00 kg/hr
	1stProd Draw Rate Draw Flow Basis Spec Value	Estimate 1stProd Molar 68.00 kgmole/hr
Parameters [Solver]	Damping Factor Fixed	0.25
	Azeotrope Check	ON

4. Click the **Run** button to solve the column.

C1.3.3 Draw Stream Location

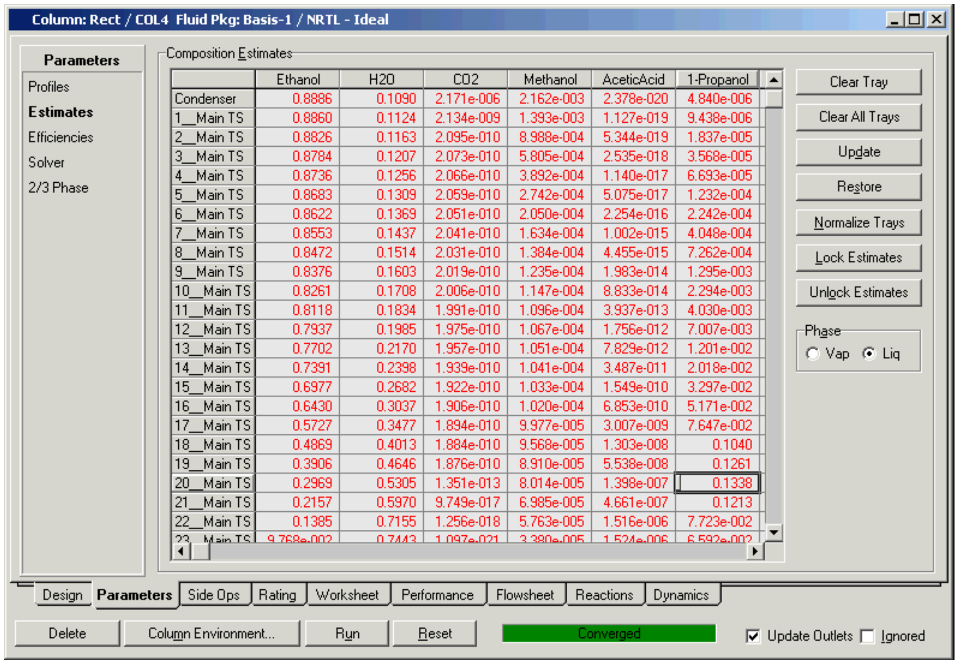
The side liquid draw, Fusel, is added at stage 20. To determine if this is an appropriate stage to recover the heavy alcohols, view the stage-by-stage composition profile.

1. To examine this information, click the **Parameters** tab in the

Column property view.

2. Select the **Estimates** page. In this view you can see the Composition Estimates of each tray.

Figure C1.5



	Ethanol	H2O	CO2	Methanol	AceticAcid	1-Propanol
Condenser	0.8886	0.1090	2.171e-006	2.162e-003	2.378e-020	4.840e-006
1__Main TS	0.8860	0.1124	2.134e-009	1.393e-003	1.127e-019	9.438e-006
2__Main TS	0.8826	0.1163	2.095e-010	8.988e-004	5.344e-019	1.837e-005
3__Main TS	0.8784	0.1207	2.073e-010	5.805e-004	2.535e-018	3.568e-005
4__Main TS	0.8736	0.1256	2.066e-010	3.892e-004	1.140e-017	6.693e-005
5__Main TS	0.8683	0.1309	2.059e-010	2.742e-004	5.075e-017	1.232e-004
6__Main TS	0.8622	0.1369	2.051e-010	2.050e-004	2.254e-016	2.242e-004
7__Main TS	0.8553	0.1437	2.041e-010	1.634e-004	1.002e-015	4.048e-004
8__Main TS	0.8472	0.1514	2.031e-010	1.384e-004	4.455e-015	7.262e-004
9__Main TS	0.8376	0.1603	2.019e-010	1.235e-004	1.983e-014	1.295e-003
10__Main TS	0.8261	0.1708	2.006e-010	1.147e-004	8.833e-014	2.294e-003
11__Main TS	0.8118	0.1834	1.991e-010	1.096e-004	3.937e-013	4.030e-003
12__Main TS	0.7937	0.1985	1.975e-010	1.067e-004	1.756e-012	7.007e-003
13__Main TS	0.7702	0.2170	1.957e-010	1.051e-004	7.829e-012	1.201e-002
14__Main TS	0.7391	0.2398	1.939e-010	1.041e-004	3.487e-011	2.018e-002
15__Main TS	0.6977	0.2682	1.922e-010	1.033e-004	1.549e-010	3.297e-002
16__Main TS	0.6430	0.3037	1.906e-010	1.020e-004	6.853e-010	5.171e-002
17__Main TS	0.5727	0.3477	1.894e-010	9.977e-005	3.007e-009	7.647e-002
18__Main TS	0.4869	0.4013	1.884e-010	9.568e-005	1.303e-008	0.1040
19__Main TS	0.3906	0.4646	1.876e-010	8.910e-005	5.538e-008	0.1261
20__Main TS	0.2969	0.5305	1.351e-013	8.014e-005	1.398e-007	0.1338
21__Main TS	0.2157	0.5970	9.749e-017	6.985e-005	4.661e-007	0.1213
22__Main TS	0.1385	0.7155	1.256e-018	5.763e-005	1.516e-006	7.723e-002
23__Main TS	9.768e-002	0.7443	1.097e-021	3.380e-005	1.524e-006	6.592e-002

3. To view the 1-Propanol composition on Tray 20, scroll through the group until you can see Tray 20 and the 1-Propanol component.

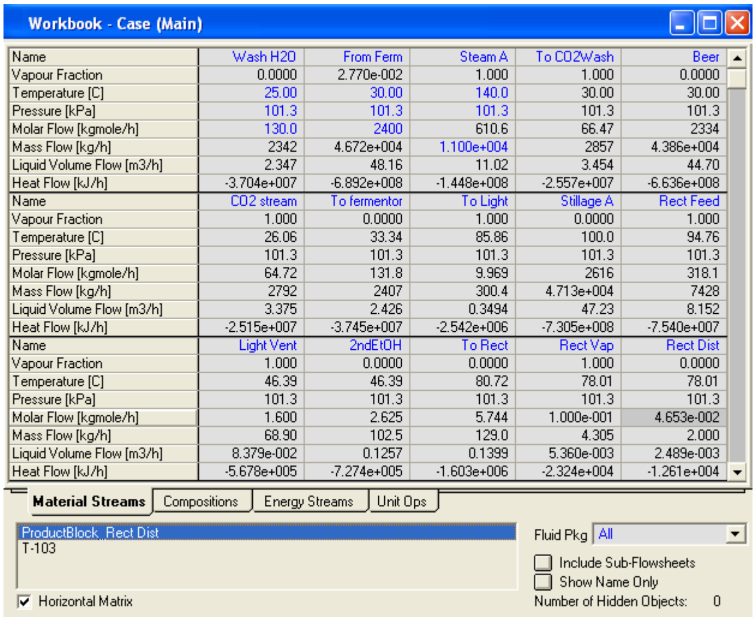
Stage 20 has a high concentration of 1-Propanol (which has the greatest concentration among the heavy alcohols). Therefore, we have selected the appropriate stage for the Fusel draw.

C1.4 Results

Workbook Case (Main)

Material Streams Tab

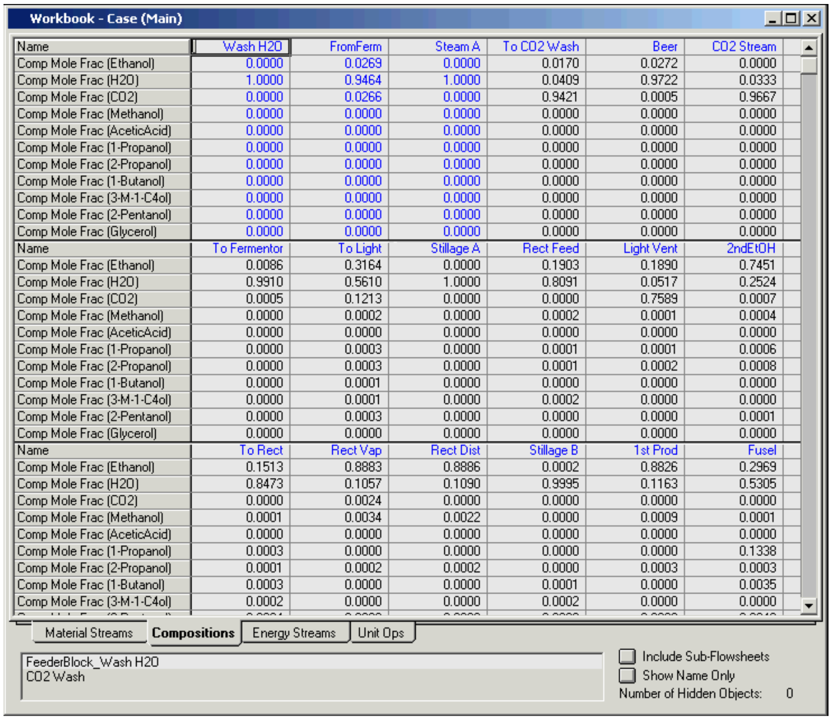
Figure C1.6



Name	Wash H20	From Ferm	Steam A	To CO2Wash	Beer
Vapour Fraction	0.0000	2.770e-002	1.000	1.000	0.0000
Temperature [C]	25.00	30.00	140.0	30.00	30.00
Pressure [kPa]	101.3	101.3	101.3	101.3	101.3
Molar Flow [kgmole/h]	130.0	2400	610.6	66.47	2334
Mass Flow [kg/h]	2342	4.672e+004	1.100e+004	2857	4.386e+004
Liquid Volume Flow [m3/h]	2.347	48.16	11.02	3.454	44.70
Heat Flow [kJ/h]	-3.704e+007	-6.892e+008	-1.448e+008	-2.557e+007	-6.636e+008
Name	CO2 stream	To fermentor	To Light	Stillage A	Rect Feed
Vapour Fraction	1.000	0.0000	1.000	0.0000	1.000
Temperature [C]	26.06	33.34	85.86	100.0	94.76
Pressure [kPa]	101.3	101.3	101.3	101.3	101.3
Molar Flow [kgmole/h]	64.72	131.8	9.969	2616	318.1
Mass Flow [kg/h]	2792	2407	300.4	4.713e+004	7428
Liquid Volume Flow [m3/h]	3.375	2.426	0.3494	47.23	8.152
Heat Flow [kJ/h]	-2.515e+007	-3.745e+007	-2.542e+006	-7.305e+008	-7.540e+007
Name	Light Vent	2ndEtOH	To Rect	Rect Vap	Rect Dist
Vapour Fraction	1.000	0.0000	0.0000	1.000	0.0000
Temperature [C]	46.39	46.39	80.72	78.01	78.01
Pressure [kPa]	101.3	101.3	101.3	101.3	101.3
Molar Flow [kgmole/h]	1.600	2.625	5.744	1.000e-001	4.653e-002
Mass Flow [kg/h]	68.90	102.5	129.0	4.305	2.000
Liquid Volume Flow [m3/h]	8.379e-002	0.1257	0.1399	5.360e-003	2.489e-003
Heat Flow [kJ/h]	-5.678e+005	-7.274e+005	-1.603e+006	-2.324e+004	-1.261e+004

Compositions Tab

Figure C1.7

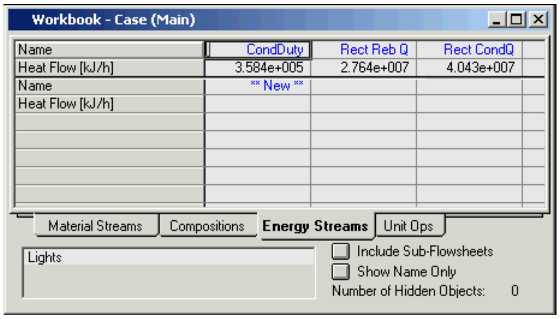


Workbook - Case (Main)

Name	Wash H2O	FromFerm	Steam A	To CO2 Wash	Beer	CO2 Stream
Comp Mole Frac (Ethanol)	0.0000	0.0269	0.0000	0.0170	0.0272	0.0000
Comp Mole Frac (H2O)	1.0000	0.9464	1.0000	0.0409	0.9722	0.0333
Comp Mole Frac (CO2)	0.0000	0.0266	0.0000	0.9421	0.0005	0.9667
Comp Mole Frac (Methanol)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (AceticAcid)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (1-Propanol)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (2-Propanol)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (1-Butanol)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (3-M-1-C4ol)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (2-Pentanol)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Glycerol)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Name	To Fermentor	To Light	Stillage A	Rect Feed	Light Vent	2ndEtOH
Comp Mole Frac (Ethanol)	0.0086	0.3164	0.0000	0.1903	0.1890	0.7451
Comp Mole Frac (H2O)	0.9910	0.5610	1.0000	0.8091	0.0517	0.2524
Comp Mole Frac (CO2)	0.0005	0.1213	0.0000	0.0000	0.7589	0.0007
Comp Mole Frac (Methanol)	0.0000	0.0002	0.0000	0.0002	0.0001	0.0004
Comp Mole Frac (AceticAcid)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (1-Propanol)	0.0000	0.0003	0.0000	0.0001	0.0001	0.0006
Comp Mole Frac (2-Propanol)	0.0000	0.0003	0.0000	0.0001	0.0002	0.0008
Comp Mole Frac (1-Butanol)	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (3-M-1-C4ol)	0.0000	0.0001	0.0000	0.0002	0.0000	0.0000
Comp Mole Frac (2-Pentanol)	0.0000	0.0003	0.0000	0.0000	0.0000	0.0001
Comp Mole Frac (Glycerol)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Name	To Rect	Rect Vap	Rect Dist	Stillage B	1st Prod	Fusel
Comp Mole Frac (Ethanol)	0.1513	0.8883	0.8886	0.0002	0.8826	0.2969
Comp Mole Frac (H2O)	0.8473	0.1057	0.1090	0.9995	0.1163	0.5305
Comp Mole Frac (CO2)	0.0000	0.0024	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Methanol)	0.0001	0.0034	0.0022	0.0000	0.0009	0.0001
Comp Mole Frac (AceticAcid)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (1-Propanol)	0.0003	0.0000	0.0000	0.0000	0.0000	0.1338
Comp Mole Frac (2-Propanol)	0.0001	0.0002	0.0002	0.0000	0.0003	0.0003
Comp Mole Frac (1-Butanol)	0.0003	0.0000	0.0000	0.0001	0.0000	0.0035
Comp Mole Frac (3-M-1-C4ol)	0.0002	0.0000	0.0000	0.0002	0.0000	0.0000

Energy Streams Tab

Figure C1.8



Workbook - Case (Main)

Name	CondDuty	Rect Reb Q	Rect CondQ
Heat Flow [kJ/h]	3.584e+005	2.764e+007	4.043e+007
Name	** New **		
Heat Flow [kJ/h]			

C2 Synthesis Gas Production

C2.1 Process Description **2**

C2.2 Setup **3**

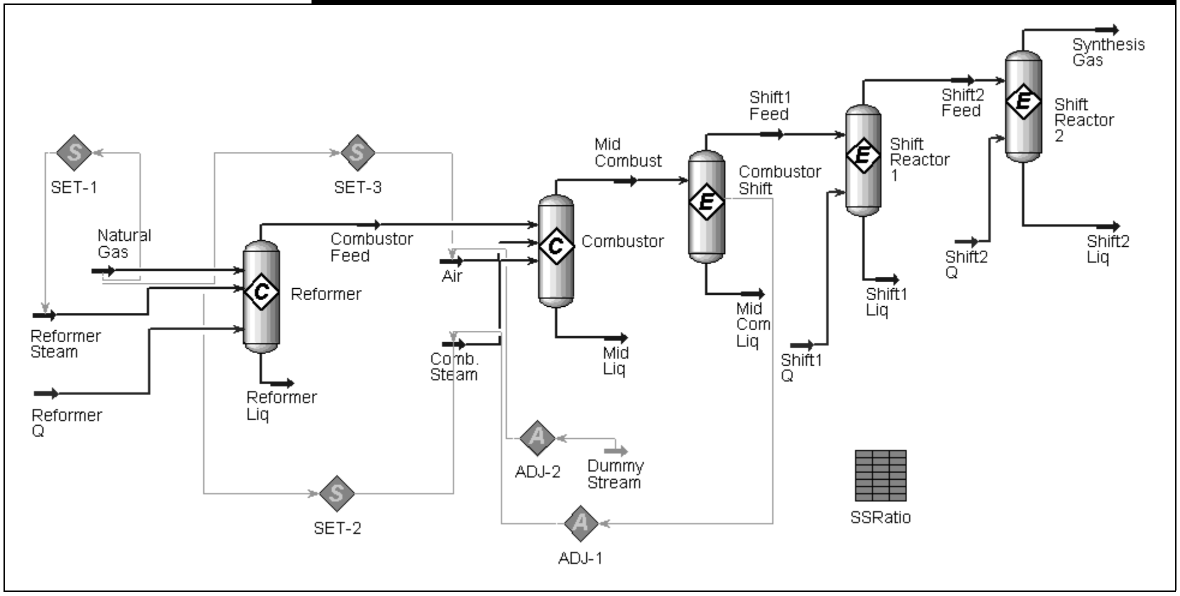
C2.3 Steady State Simulation **6**

C2.3.1 Building the Flowsheet 6
C2.3.2 Installing Adjust Operations 9

C2.4 Results **11**

C2.1 Process Description

Figure C2.1



The production of synthesis gas is an important part of the overall process of synthesizing ammonia. The conversion of natural gas into the feed for the ammonia plant is modeled using three conversion reactions and an equilibrium reaction. To facilitate the production of ammonia, the molar ratio of hydrogen to nitrogen in the synthesis gas is controlled near 3:1. This ratio represents the stoichiometric amounts of the reactants in the ammonia process.

In a typical synthesis gas process, four reactors are needed. This model requires five reactors since the conversion and equilibrium reactions cannot be placed in the same reaction set and thus cannot be placed in the same reactor. The Combustor is separated into a conversion reactor and an equilibrium reactor.

Desulfurized natural gas is the source of hydrogen in this example, which is reformed in a conversion reactor (Reformer) when combined with steam. Air is added to the second reactor at a controlled flow rate such that the desired ratio of H2:N2 in the synthesis gas is attained.

The oxygen from the air is consumed in an exothermic combustion reaction while the inert nitrogen passes through the system. The addition of steam serves the dual purpose of maintaining the reactor temperature and ensuring that the excess methane from the natural gas stream is consumed. In the last two reactors, the water-gas shift equilibrium reaction takes place as the temperature of the stream is

successively lowered.

There are two general steps in this process simulation:

1. **Setup**. In this step the Fluid package, Reaction sets and Reaction components are selected. The Reaction Component list includes CH4, H2O, CO, CO2, H2, N2 and O2.
2. **Steady State Simulation**. The case will be built in steady state with the following key unit ops:
   - **Reformer**. A conversion reactor in which most of the methane is reacted with steam to produce hydrogen, carbon monoxide and carbon dioxide.
   - **Combustor**. A second conversion reactor, which takes the product of the Reformer, an Air stream and a Comb. Steam stream as the feeds to the reactor.
   - **Shift Reactors**. A series of equilibrium reactors in which the water gas shift reaction occurs.

C2.2 Setup

1. In the Session Preferences view, select **Field** unit set for this application.
2. In the Component List view, select the following components: **methane**, **water**, **carbon monoxide**, **carbon dioxide**, **hydrogen**, **nitrogen**, and **oxygen**.
3. In the Fluid Package view, select the **Peng-Robinson** property package.
4. Go to the **Rxns** tab, and add the **Global Rxn Set** to the current reaction sets.

Defining the Reactions

Refer to **Chapter 5 - Reactions** in the **UniSim Design Simulation Basis Guide** for more information about how to define reactions and reaction sets.

In this application, there are three conversion reactions and one equilibrium reaction.

Conversion Reactions

The reforming reactions are as follows:

$$CH_4 + H_2O \rightarrow CO + 3H_2 \quad (C2.1)$$

$$CH_4 + 2H_2O \rightarrow CO_2 + 4H_2 \quad (C2.2)$$

The combustion reaction is as follows:

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O \qquad (C2.3)$$

Equilibrium Reaction

The water-gas shift reaction is as follows:

$$CO + H_2O \leftrightarrow CO_2 + H_2 \qquad (C2.4)$$

The **Rxn Components** group only shows the components associated with the Fluid Package(s).

To add or edit components, select the Add Comps button. The new components will automatically be added to any fluid package that uses the reaction.

To define the reaction:

1. In the Simulation Basis Manager view, go to the **Reactions** tab.

   The reaction components are attached based on the associated fluid package and are listed in the Rxn Components group.

2. Add the two reforming reactions using the following data:

Reaction [Rxn-1]		
Reactions View	**Type**	**Conversion**
Tab	**In this cell...**	**Enter...**
Stoichiometry	**Component (Stoich. Coeff.)**	Methane (-1)
		Water (-1)
		CO (1)
		Hydrogen (3)
Basis	**Base Component**	Methane
	Rxn Phase	VaporPhase
	Conversion	40% (Co)
Comments	CH4 + H2O g CO + 3H2	

Reaction [Rxn-2]		
Reactions View	**Type**	**Conversion**
Tab	**In this cell...**	**Enter...**
Stoichiometry	**Component (Stoich. Coeff.)**	Methane (-1)
		Water (-2)
		CO2 (1)
		Hydrogen (4)
Basis	**Base Component**	Methane
	Rxn Phase	VaporPhase
	Conversion	30% (Co)
Comments	CH4 + 2H2O g CO2 + 4H2	

3. Add the combustion reaction using the following data:

Reaction [Rxn-3]		
Reactions View	**Type**	**Conversion**
Tab	**In this cell...**	**Enter...**
Stoichiometry	**Component (Stoich. Coeff.)**	Methane (-1)
		Oxygen (-2)
		CO2 (1)
		Water (2)
Basis	**Base Component**	Methane
	Rxn Phase	VaporPhase
	Conversion	100%
Comments	CH4 + 2O2 g CO2 + 2H2O	

UniSim Design contains a library of equilibrium reactions. To add the equilibrium reaction:

4. On the Reactions view, select **Equilibrium** and click the **Add Reaction** button.
5. In the Equilibrium Reaction view, go to the **Library** tab, select **CO + H2O = CO2 + H2**, and click the **Add Library Rxn** button.

   UniSim Design provides the equilibrium data and all other pertinent information for the reaction.

Defining Reaction Sets

In the table of reaction sets, RXN-1 and RXN-2 appear in both the first and second reaction sets.

In UniSim Design, each reactor operation may have only one reaction set attached to it, however, a reaction may appear in multiple reaction sets. In this case, you only have to provide three reaction sets for all five reactors.

1. On the **Reactions** tab of the Simulation Basis Manager view, click the **Add Set** button to add new reaction sets. Define the following reactions sets:

Reaction Set Name	Active Reactions
Reformer Rxn Set	Rxn-1, Rxn-2
Combustor Rxn Set	Rxn-1, Rxn-2, Rxn-3
Shift Rxn Set	Rxn-4

To attach the reaction sets to the Fluid Package:

2. On the **Reactions** tab of the Simulation Basis Manager, select a Reaction Set and click the **Add to FP** button.

3. In the Add view, select a fluid package from the list and click the **Add Set to Fluid Package** button. Repeat the procedure for the other two reaction sets.

C2.3 Steady State Simulation

Installing Streams

Here you will define the two feed streams to the first reactor (Natural Gas and Reformer Steam). The Comb. Steam stream and the Air stream will also be defined. The pressures of the steam and air streams will be specified later using SET operations. Install and define the streams as indicated.

Name	Natural Gas	Reformer Steam	Air	Comb. Steam
Temperature[F]	700.0	475.0	60.0	475.0
Pressure [psia]	500.0	<empty>	<empty>	<empty>
Molar Flow [lbmole/hr]	200.0	520.0	200.0**	300.0**
Comp Mole Frac [CH4]	1.0000	0.0000	0.0000	0.0000
Comp Mole Frac [H2O]	0.0000	1.0000	0.0000	1.0000
Comp Mole Frac [CO]	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac [CO2]	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac [H2]	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac [N2]	0.0000	0.0000	0.7900	0.0000
Comp Mole Frac [O2]	0.0000	0.0000	0.2100	0.0000
COMMENTS: ** signifies initialized values; the molar flows of **Air** and **Comb. Steam** will be manipulated by **Adjust-2** and **Adjust-1** respectively.				

C2.3.1 Building the Flowsheet

Set Operations

An alternative method for setting the steam and air pressures is to import the Natural Gas pressure to a Spreadsheet, copy the value for each of the other streams and export the copied values to the streams

Install the following Set operations to specify the pressures of the steam and air streams. Install these before installing the Reformer so the reactor is calculated when you install it.

Set [SET-1]		
Tab	**In this cell...**	**Enter...**
Connections	Target Object	Reformer Steam
	Target Variable	Pressure
	Source Object	Natural Gas
Parameters	Multiplier	1
	Offset	0

Set [SET-2]		
Tab	**In this cell...**	**Enter...**
Connections	Target Object	Comb. Steam
	Target Variable	Pressure
	Source Object	Natural Gas
Parameters	Multiplier	1
	Offset	0

Set [SET-3]		
Tab	**In This Cell...**	**Enter**
Connections	Target Object	Air
	Target Variable	Pressure
	Source Object	Natural Gas
Parameters	Multiplier	1
	Offset	0

Installing the Reformer

The Reformer is a conversion reactor in which most of the methane is reacted with steam to produce hydrogen, carbon monoxide, and carbon dioxide. The outlet gas will also contain the unreacted methane and excess water vapour from the steam. The overall conversion of the two reactions in the Reformer is 70%. Rxn-1, which produces carbon monoxide and hydrogen, has a conversion of 40%, while Rxn-2 has a conversion rate of 30%.

The two reforming reactions are endothermic, so heat must be supplied to the reactor to maintain the reactor temperature. Specify the temperature of the outlet stream, Combustor Feed, at 1700 °F, so that UniSim Design will calculate the required duty.

Install the reactor and define it as indicated below.

Conversion Reactor [Reformer]		
Tab [Page]	**In this cell...**	**Enter...**
Design [Connections]	Inlets	Natural Gas
		Reformer Steam
	Vapour Outlet	Combustor Feed
	Liquid Outlet	Reformer Liq
	Energy	Reformer Q
Design [Parameters]	Optional Heat Transfer	Heating
Worksheet [Conditions]	Combustor Feed Temperature	1700 °F
Reactions [Details]	Reaction Set	Reformer Rxn Set
Comments	CH4 + H2O g CO + 3H2	
	CH4 + 2H2O g CO2 + 4H2	

Installing the Combustor

This reactor is adiabatic, so there is no energy stream and you do not have to specify the outlet temperature.

The Combustor is the second conversion reactor. The feed streams for the Combustor include the Reformer product, Air stream and Comb. Steam streams. The air stream is the source of the nitrogen for the required H2:N2 ratio in the synthesis end product. The oxygen in the air is consumed in the combustion of methane. Any remaining methane in the Combustor is eliminated by this reaction.

UniSim Design automatically ranks the three reactions in the Combustor Rxn Set. Since H2O is a reactant in the combustion reaction (Rxn-1) and is a product in the two reforming reactions (Rxn-2 and Rxn-3), UniSim Design provides a lower rank for the combustion reaction. An equal rank is given to the reforming reactions. With this ranking, the combustion reaction proceeds until its specified conversion is met or a limiting reactant is depleted. The reforming reactions then proceed based on the remaining methane.

Reactions of equal ranking can have an overall specified conversion between 0% and 100%.

Install the Combustor and define it as indicated below.

Conversion Reactor [Combustor]		
Tab [Page]	**In this cell...**	**Enter...**
Design [Connections]	Inlets	Combustor Feed
		Air
		Comb. Steam
	Vapour Outlet	Mid Combust
	Liquid Outlet	Mid Liq
Reactions [Details]	Reaction Set	Combustor Rxn Set
	Rxn-1 Conversion	35%
	Rxn-2 Conversion	65%
	Rxn-3 Conversion	100%
Comments	CH4 + H2O g CO + 3H2	
	CH4 + 2H2O g CO2 + 4H2	
	CH4 + 2O2 g CO2 + 2H2O	

Shift Reactors

The three shift reactors are all equilibrium reactors within which the water-gas shift reaction occurs. In the Combustor Shift reactor, the equilibrium shift reaction takes place and would occur with the reactions in the Combustor. A separate reactor must be used in the model because equilibrium and conversion reactions cannot be combined within a reaction set.

Install the following three equilibrium reactors as shown below:

Equilibrium Reactor [Combustor Shift]		
Tab [Page]	**In this cell...**	**Enter...**
Design [Connections]	Inlets	Mid Combust
	Vapour Outlet	Shift1 Feed
	Liquid Outlet	Mid Com Liq
Reactions [Details]	Reaction Set	Shift Rxn Set
Comments	Reaction: $CO + H_2O$ n $CO_2 + H_2$	

Equilibrium Reactor [Shift Reactor 1]		
Tab [Page]	**In this cell...**	**Enter...**
Design [Connections]	Inlets	Shift1 Feed
	Vapour Outlet	Shift2 Feed
	Liquid Outlet	Shift1 Liq
	Energy	Shift1 Q
Design [Parameters]	Optional Heat Transfer	Cooling
Worksheet [Conditions]	Shift2 Feed Temperature	850°F
Reactions [Details]	Reaction Set	Shift Rxn Set
Comments	Reaction: $CO + H_2O$ n $CO_2 + H_2$	

Equilibrium Reactor [Shift Reactor 2]		
Tab [Page]	**In this cell...**	**Enter...**
Design [Connections]	Feeds	Shift2 Feed
	Vapour Outlet	Synthesis Gas
	Liquid Outlet	Shift2 Liq
	Energy	Shift2 Q
Design [Parameters]	Optional Heat Transfer	Cooling
Worksheet [Conditions]	Synthesis Gas Temperature	750°F
Reactions [Details]	Reaction Set	Shift Rxn Set
Comments	Reaction: $CO + H_2O$ n $CO_2 + H_2$	

C2.3.2 Installing Adjust Operations

Steam flow Rate

To control the temperature of the combustion reaction, the flow rate of steam to the Combustor is adjusted. Since the Combustor is modeled as two separate reactors, the temperature of the equilibrium reactor (Combustor Shift) is targeted.

The same Adjust could be accomplished by selecting the temperature of the stream Shift1 Feed.

An ADJUST operation is used to manipulate the Comb. Steam flow rate

to maintain the Combustor Shift temperature at 1700°F.

Adjust [ADJ-1]		
Tab	**In this cell...**	**Enter...**
Connections	**Adjusted Object**	Comb. Steam
	Adjusted Variable	Molar Flow
	Target Object	Combustor Shift
	Target Variable	Vessel Temp.
	Spec. Target Value	1700°F
Parameters	**Method**	Secant
	Tolerance	0.1°F
	Step Size	50 lbmole/hr
	Maximum Iterations	25

Click the **Start** button to begin the Adjust operation.

Air Flow Rate

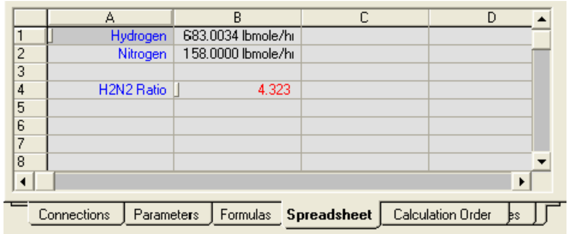
To control the H2:N2 molar ratio in the Synthesis Gas stream, calculate the ratio in a Spreadsheet and then use an Adjust operation. The Synthesis Gas should have an H2:N2 molar ratio slightly greater than 3:1. Prior to entering the ammonia plant, hydrogen is used to rid the synthesis gas of any remaining CO and CO2.

1. Create a Spreadsheet and change the Spreadsheet Name to **SSRatio**. Import the following variables:
   - Synthesis Gas, Comp. Molar Flow, Hydrogen
   - Synthesis Gas, Comp. Molar Flow, Nitrogen
2. Assign the Hydrogen value to cell B1, and the Nitrogen value to cell B2.
3. In cell B4, calculate the H2:N2 ratio using the following formula:

   =B1[cell that contains flow of H2]/B2[cell that contains flow of N2]

   The Spreadsheet tab of the Spreadsheet view should appear similar to the following.

Figure C2.2



4. Click the **Parameters** tab and define the **Variable** name for the B4 cell as H2:N2 Ratio.
5. Install the Adjust operation as shown below.

Adjust [ADJ-2]		
Tab	**In this cell...**	**Enter...**
Connections	Adjusted Variable	Air Molar Flow
	Target Variable	SSRatio, B4: H2:N2 Ratio
	Spec. Target Value	3.05
Parameters	Method	Secant
	Tolerance	0.005 lbmole/hr
	Step Size	39.68 lbmole/hr
	Maximum Iterations	20

6. Click the **Start** button to begin the Adjust operation.

   The Secant method is used for both Adjust operations even though each adjusted variable will have an effect on the other operation's target variable. The close proximity of the logical operations in the flowsheet increases the possibility of cycling behaviour if the Simultaneous method is used. Therefore, it is advantageous to attempt to iterate on one Adjust and then solve the other.

C2.4 Results

Go to the Workbook in the main simulation environment to check the calculated results.

Energy Streams Tab

Figure C2.3

Name	Reformer Q	Shift1 Q	Shift2 Q
Heat Flow [Btu/hr]	2.238e+007	7.349e+006	1.282e+006

Material Streams Tab

Figure C2.4

Name	Natural Gas	Reformer Stean	Air	Comb. Steam	Combustor Feec	Reformer Liq	Mid Combust
Vapour Fraction	1.0000	1.0000	1.0000	1.0000	1.0000	0.0000	1.0000
Temperature [F]	700.0	475.0	60.00	475.0	1700	1700	1479
Pressure [psia]	500.0	500.0	500.0	500.0	500.0	500.0	500.0
Molar Flow [lbmole/hr]	200.0	520.0	107.2	55.22	1000	0.0000	1260
Mass Flow [lb/hr]	3209	9368	3092	994.8	1.258e+004	0.0000	1.666e+004
Liquid Volume Flow [barrel/day]	733.8	642.7	244.7	68.26	1975	0.0000	2502
Heat Flow [Btu/hr]	-5.115e+006	-5.254e+007	-2.574e+004	-5.580e+006	-3.528e+007	0.0000	-4.088e+007
Name	Mid Liq	Shift1 Feed	Mid Com Liq	Shift2 Feed	Shift1 Liq	Synthesis Gas	Shift2 Liq
Vapour Fraction	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000
Temperature [F]	1479	1440	1440	850.0	850.0	750.0	750.0
Pressure [psia]	500.0	500.0	500.0	500.0	500.0	500.0	500.0
Molar Flow [lbmole/hr]	0.0000	1260	0.0000	1260	0.0000	1260	0.0000
Mass Flow [lb/hr]	0.0000	1.666e+004	0.0000	1.666e+004	0.0000	1.666e+004	0.0000
Liquid Volume Flow [barrel/day]	0.0000	2447	0.0000	2590	0.0000	2620	0.0000
Heat Flow [Btu/hr]	0.0000	-4.088e+007	0.0000	-4.823e+007	0.0000	-4.951e+007	0.0000
Name	** New **						

Material Streams | Compositions | Energy Streams | Unit Ops

Compositions Tab

Figure C2.5

Name	Natural Gas	Reformer Stean	Air	Comb. Steam	Combustor Feec	Reformer Liq	Mid Combust
Comp Mole Frac (Methane)	1.0000	0.0000	0.0000	0.0000	0.0600	0.0600	0.0000
Comp Mole Frac (H2O)	0.0000	1.0000	0.0000	1.0000	0.3200	0.3200	0.2518
Comp Mole Frac (CO)	0.0000	0.0000	0.0000	0.0000	0.0800	0.0800	0.0770
Comp Mole Frac (CO2)	0.0000	0.0000	0.0000	0.0000	0.0600	0.0600	0.0817
Comp Mole Frac (Hydrogen)	0.0000	0.0000	0.0000	0.0000	0.4800	0.4800	0.5222
Comp Mole Frac (Nitrogen)	0.0000	0.0000	0.7900	0.0000	0.0000	0.0000	0.0672
Comp Mole Frac (Oxygen)	0.0000	0.0000	0.2100	0.0000	0.0000	0.0000	0.0000
Name	Mid Liq	Shift1 Feed	Mid Com Liq	Shift2 Feed	Shift1 Liq	Synthesis Gas	Shift2 Liq
Comp Mole Frac (Methane)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (H2O)	0.2518	0.2738	0.2737	0.2171	0.2172	0.2049	0.2051
Comp Mole Frac (CO)	0.0770	0.0990	0.0990	0.0423	0.0423	0.0301	0.0301
Comp Mole Frac (CO2)	0.0817	0.0598	0.0598	0.1164	0.1165	0.1286	0.1286
Comp Mole Frac (Hydrogen)	0.5222	0.5003	0.5003	0.5570	0.5568	0.5691	0.5689
Comp Mole Frac (Nitrogen)	0.0672	0.0672	0.0672	0.0672	0.0672	0.0672	0.0672
Comp Mole Frac (Oxygen)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Name	** New **						

Material Streams | **Compositions** | Energy Streams | Unit Ops

X1 Case Linking

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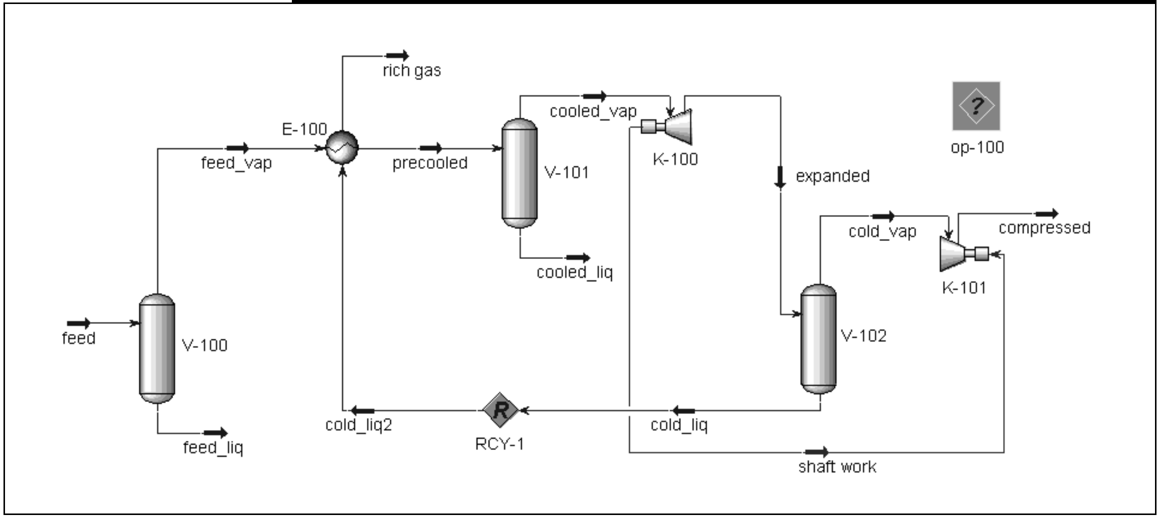
X1.1 Process Description

This example uses the User Unit Operation to link two UniSim Design cases together such that changes made to the first case (LinkCase1) are automatically and transparently propagated to the second (LinkCase2). This application demonstrates a method for copying the contents of a stream from one case to another automatically.

Figure X1.1



The User Unit Op is pre-configured with Visual Basic™ code. Inside the User Unit Op you will define two subroutines:

- **Initialize()** macro. The Initialize() macro sets the field names for the various stream feed and product connections and creates the following two text user variables:
  - **LinkCase** contains the path and file name of the target case to be linked. If the variable contains no value, the Initialize() code will set it to be the path to the currently open case and the file name **LinkCase2.usc**.
  - **LinkStream** names a stream in the second case that will have the T, P, Flow and composition copied to it from the User Unit Op's feed stream. The target case and stream may optionally be changed explicitly from the Variables page of the User Unit Op.
- **Execute()** macro. The Execute() macro uses the GetObject method to open the target link case, which will initially be hidden. It then attempts to locate the material stream named by the LinkStream variable in the target case. If a stream is

All the stream names are in **lower case**.

attached to the Feeds1 nozzle of the User Unit Op, the stream conditions and compositions are then copied between the streams.

The use of the DuplicateFluid method to copy the stream parameters requires identical property packages in both simulation cases. The example code instead uses a technique of explicitly copying T and P and then searches for components by name in order to copy their molar flow. Components that are not available in the target case are ignored.

Also, the definition of User Unit Op usually involves the definition of three macros:

- **Initialize()**
- **Execute()**
- **StatusQuery()**

For this example, the StatusQuery() macro is commented-out to avoid the overhead of having that macro called. Removing the StatusQuery() code entirely would accomplish the same thing, but it is highly recommended that StatusQuery() be implemented to provide valuable user feedback. This implementation is left as an exercise for the user.

X1.2 Building Flowsheet 1

X1.2.1 Setup

1. In the Session Preferences view, set the unit set to **SI**.
2. In the Component List view, select the following components: **C1**, **C2**, **C3**, and **i-C4**.
3. In the Fluid Package view, define a Peng Robinson Stryjek Vera (**PRSV**) property package.

X1.2.2 Installing Streams

Enter the Simulation Environment and specify streams **feed** and **cold_liq2** as shown.

Stream Name	feed	cold_liq2
In this cell...	**Enter...**	**Enter...**
Temperature [C]	11	-98
Pressure [kPa]	5066	152
Molar Flow [kgmole/h]	100	7.5

Stream Name	feed	cold_liq2
Comp Mole Frac [C1]	0.5333	0.0388
Comp Mole Frac [C2]	0.2667	0.4667
Comp Mole Frac [C3]	0.1333	0.3883
Comp Mole Frac [i-C4]	0.0667	0.1062

X1.2.3 Installing Unit Operations

Next add the following unit operations to the flowsheet.

Add Separators

Separator Name	V-100	
Tab [Page]	**In this cell...**	**Enter...**
Design [Connections]	Inlet	feed
	Vapour Outlet	feed_vap
	Liquid Outlet	feed_liq
Design [Parameters]	Delta P	0 kPa
	V-101	
Tab [Page]	**In this cell...**	**Enter...**
Design [Connections]	Inlet	precooled
	Vapour Outlet	cooled_vap
	Liquid Outlet	cooled_liq
Design [Parameters]	Delta P	0 kPa
	V-102	
Tab [Page]	**In this cell...**	**Enter...**
Design [Connections]	Inlet	expanded
	Vapour Outlet	cold_vap
	Liquid Outlet	cold_liq
Design [Parameters]	Delta P	0 kPa

Add a Heat Exchanger

Heat Exchanger Name	E-100	
Tab [Page]	**In this cell...**	**Enter...**
Design [Connections]	Tube Side Inlet	feed_vap
	Tube Side Outlet	precooled
	Shell Side Inlet	cold_liq2
	Shell Side Outlet	rich gas

Heat Exchanger Name	E-100	
Design [Parameters]	Heat Exchanger Model	Exchanger Design (End Point)
	Heat Leak/Loss	none
	Tube Side Delta P	15 kPa
	Shell Side Delta P	15 kPa
	UA	4000 KJ/C-h
Rating [Sizing]	First Tube Pass Flow Direction	Counter

Add an Expander

Expander Name	K-100	
Tab [Page]	**In this cell...**	**Enter...**
Design [Connections]	Inlet	cooled_vap
	Outlet	expanded
	Energy	shaft work
Design [Parameters]	Efficiency (Adiabatic)	75%
Worksheet [Conditions]	Pressure (stream: expanded)	152 kPa

Add a Compressor

Compressor Name	K-101	
Tab [Page]	**In this cell...**	**Enter...**
Design [Connections]	Inlet	cold_vap
	Outlet	compressed
	Energy	shaft work
Design [Parameters]	Efficiency (Adia)	75%

Add a Recycle Operation

Recycle	RCY-1	
Tab [Page]	**In this cell...**	**Enter...**
Design [Connections]	Inlet	cold_liq
	Outlet	cold_liq2

The case should converge immediately.

Save the case as **LinkCase1.usc**.

X1.3 Building Flowsheet 2

X1.3.1 Setup

Now you will create the target case for the linked case.

1. In the Session Preferences view, set the unit set to **SI**.
2. In the Component List view, select the following components: **C1**, **C2**, **C3**, **i-C4**, and **H2O**.
3. In the Fluid Package view, define a Peng Robinson Stryjek Vera (**PRSV**) property package.

X1.3.2 Installing Unit Operations

Enter the Simulation Environment and enter the following unit operations.

Add Compressors

Compressor Name	K-100	
Tab [Page]	**In this cell...**	**Enter...**
Design [Connections]	Inlet	compressed
	Outlet	hot33atm
	Energy	q1
Design [Parameters]	Efficiency (Adia)	75%
Worksheet [Conditions]	Pressure (stream: hot33atm)	3344.725 kPa
	K-101	
Tab [Page]	**In this cell...**	**Enter...**
Design [Connections]	Inlet	cool33atm
	Outlet	hot100atm
	Energy	q2
Design [Parameters]	Efficiency (Adia)	75%
Worksheet [Conditions]	Pressure (stream: hot100atm)	10150 kPa

Add Heat Exchangers

Heat Exchanger Name	E-100	
Tab [Page]	**In this cell...**	**Enter...**

Heat Exchanger Name	E-100	
Design [Connections]	Tube Side Inlet	hot33atm
	Tube Side Outlet	cool33atm
	Shell Side Inlet	wtr1
	Shell Side Outlet	wtr1b
Design [Parameters]	Heat Exchanger Model	Exchanger Design (End Point)
	Tube Side Delta P	15 kPa
	Shell Side Delta P	15 kPa
	Calculate Ft Factor	Unchecked
Rating [Sizing]	First Tube Pass Flow Direction	Counter
Worksheet [Conditions]	Temperature (stream: cool33atm)	17°C
	Temperature (stream: wtr1b)	25°C
	E-101	
Tab [Page]	**In this cell...**	**Enter...**
Design [Connections]	Tube Side Inlet	hot100atm
	Tube Side Outlet	sales
	Shell Side Inlet	wtr2
	Shell Side Outlet	wtr2b
Design [Parameters]	Heat Exchanger Model	Exchanger Design (End Point)
	Tube Side Delta P	15 kPa
	Shell Side Delta P	15 kPa
	Calculate Ft Factor	Unchecked
Rating [Sizing]	First Tube Pass Flow Direction	Counter
Worksheet [Conditions]	Temperature (stream: sales)	20°C
	Temperature (stream: wtr2b)	25°C

Add a Tee

Tee	T-100	
Tab [Page]	**In this cell...**	**Enter...**
Design [Connections]	Inlet	cooling water
	Outlet	wtr2, wtr1
Worksheet [Conditions]	Temperature (stream: cooling water)	11°C
	Pressure (stream: cooling water)	202.6 kPa
Worksheet [Composition]	H2O (stream: cooling water)	1.0000

4. Once you have completed specifying this flowsheet, save the case as **LinkCase2.usc** and close it.

X1.4 Creating a User Unit Operation

Now that both cases have been created, you can create the link between them.

1. Open **LinkCase1.usc**.
2. Add a User Unit Op to the flowsheet. When you add a User Unit Op, UniSim Design asks you for the type. Click the **Create Type** button, then type **Case Linking** in the input field and click the **OK** button.

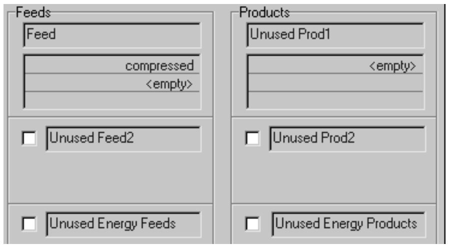
   Next you will define the User Unit Op. Defining the User Unit Op involves writing two different subroutines.

   - **Initialize.** Defines material and energy feed/product streams and creates user variables.
   - **Execute.** Opens the target case, finds the target stream and copies the stream conditions from the main case.
3. In the User Unit Op view **Design** tab, select the **Code** page.
4. Click the **Edit** button. The Edit Existing Code view appears.

X1.4.1 Initializing the User Unit Op

The following table contains a listing of the code required to implement this operation, along with a brief description of what the code means. Partitions placed in the code are made only to clearly associate the relevant code with the explanation. Also, indentations made in the code are common with standard programming practices.

Code	Explanation
`Sub Initialize ()`	Signifies the Start of the initialization subroutine. You do not have to add it as it should already be there.

`On Error GoTo Catch`
`' Preparing the interface`
`ActiveObject.Feeds1Name = "Feed"`
`ActiveObject.Products1Name = "Unused Prod1"`
`ActiveObject.Feeds2Name = "Unused Feed2"`
`ActiveObject.Products2Name = "Unused Prod2"`
	If an error occurs during the execution of this subroutine, go to the line designated 'Catch'.
	Sets the names that will be associated with the energy and material (primary and secondary) inlet and exit connections.
	

Code	Explanation

`ActiveObject.Feeds2Active = False`
`ActiveObject.Products2Active = False`
`ActiveObject.EnergyFeedsActive = False`
`ActiveObject.EnergyProductsActive = False`
	Deactivates the secondary inlet and exit connections as well as the energy inlet and exit connections. After the initialization subroutine has been successfully implemented, the checkboxes associated with the secondary material connections and energy connections should be deactivated as shown in the figure above.

`' Adding user variables`
`Dim LinkCase As Object ' This UV will hold the Linked case name`
`Set LinkCase = ActiveObject.CreateUserVariable("LinkCase", "LinkCase", uvtText, utcNullUnit,0)`
	Creates a text user variables called **LinkCase**. This will appear on the Variables page of the Design tab along with the current values. This variable holds the path and name of the linked case.

`Dim LinkStream As Object ' This UV will hold the Linked stream name` `Set LinkStream = ActiveObject.CreateUserVariable("LinkStream", "LinkStream", uvtText, utcNullUnit,0)`	Creates a text user variables called **LinkStream**. This will appear on the Variables page of the Design tab along with the current values. This variable holds the name of the stream to link to.
`LinkCase.Variable.Value = ActiveObject.SimulationCase.Path & "LinkCase2.usc"`	This sets the linked case path to be the same as the current case and sets the name to 'LinkCase2.usc'.
`Dim myFeeds As Object` `Set myFeeds = ActiveObject.Feeds1`	Declares the 'myFeeds' variable and sets it to the feed streams collection of the operation.
`' Check if a stream name is already defined` `If Not LinkStream.Variable.IsKnown Then`	Checks if a linked stream name is already defined.
`If myFeeds.Count > 0 Then` `LinkStream.Variable.Value = myFeeds.Item(0).Name`	If a feed stream is connected to the unit operation, use that stream name as the linked stream name.

`Else`
`LinkStream.Variable.Value = "feed"`
`End If`
`End If`
	If no stream is connected as feed, use the default listed stream name of 'feed'.

`Exit Sub`
`Catch:`
`MsgBox "Initialize Error"`	

`End Sub`	Signifies the end of the initialization subroutine. This line does not need to be added.

1. Once this code is entered, press the **OK** button to close the Edit Existing Code view.
2. On the **Code** page of the **Design** tab, click the **Initialize** button.
3. Select the **Connections** page of the **Design** tab. It should contain their new designations.
4. Select the **Variables** page. The LinkCase should contain the case LinkCase2, including the path. The LinkStream variable should contain 'feed'.

5. Select the **Connections** page. If the feed drop-down list is empty, the value of LinkStream variable (Variables page) should be ‘feed’.

X1.4.2 Operation Execution

1. Enter the following code in the Execution code section of the Edit Existing Code view:

Code	Explanation
`Sub Execute ()`	Signifies the Start of the operation execution subroutine. You do not have to add this line as it should already be there.
`On Error Goto EarlyGrave`	If an error occurs during the execution of this subroutine, go to the line of code designated ‘EarlyGrave’.

`Dim Status As String`
 	
`Dim LinkCase As Object`
`Set LinkCase =`
`ActiveObject.GetUserVariable("LinkCase")`
 	
`Dim LinkStream As Object ' This UV will hold the Linked stream name`
`Set LinkStream =`
`ActiveObject.GetUserVariable("LinkStream")`
	Connects the variables LinkCase and LinkStream to their corresponding user variables.

`Dim myFeeds As Object`
`Set myFeeds = ActiveObject.Feeds1`
`if myFeeds.Count <>1 Then`
`Exit Sub`
`end if`
	If the number of streams specified in the Feed list is not 1 then exit the subroutine.

`Dim Case2 As Object`
`Set Case2 =`
`GetObject(LinkCase.Variable.Value)`
	Creates a reference to the LinkCase user variable called Case2.

`Dim Case2FS As Object` `Set Case2FS = Case2.Flowsheet`	Creates a reference to the flowsheet inside Case2 (LinkCase) called Case2FS.
`Dim Case1FS As Object` `Set Case1FS = ActiveObject.Flowsheet`	Creates a reference to the current flowsheet called Case1FS.

`Dim Case2Strm As Object`
`Set Case2Strm =`
`Case2FS.MaterialStreams.Item(CStr(LinkStream.Variable.Value))`
	Creates a reference to a stream in the other case. The stream’s name is the value of the user variable LinkStream.

`Dim Case1Strm As Object` `Set Case1Strm = myFeeds.Item(0)`	Creates a reference to stream currently in the primary feed list.

`Case2Strm.TemperatureValue =`
`Case1Strm.TemperatureValue`
`Case2Strm.PressureValue =`
`Case1Strm.PressureValue`
	Sets the Temperature and Pressure values of Case2Strm to those of Case1Strm.

`Dim Case1CMFs As Variant`
`Case1CMFs =`
`Case1Strm.ComponentMolarFlowValue`
	Creates an array containing the molar flow of Case1Strm. Note that Set was not used so changes made to Case1CMFs will not affect Case1Strm.

Code	Explanation

`Dim Case2CMFs As Variant`
`Case2CMFs =`
`Case2Strm.ComponentMolarFlowValue`
	Creates an array containing the molar flow of Case2Strm. Note that Set was not used so changes made to Case2CMFs will not affect Case2Strm.

`On Error GoTo NoComp`
`Dim Comp As Object`
`i = 0`
`For Each Comp In`
`Case2FS.FluidPackage.Components`
`Case2CMFs(i) = 0.0`
`CompName = Comp.name`
`n =`
`Case1FS.FluidPackage.Components.index(Co`
`mpName)`
`Case2CMFs(i) = Case1CMFs(n)`
`NoComp:`
`i = i +1`
`Next Comp`
	For every component i in the Case2FS, you set the molar flow of component i in the Case2CMFs array to the flow of the same component in Case1CMFs array.

`On Error GoTo EarlyGrave`	
`Case2Strm.ComponentMolarFlowValue =` `Case2CMFs`	This passes the value of Case2CMFs to the Case2Strm.
`ActiveObject.SolveComplete`	Signifies the Unit Operation has solved. It is used to minimize the number of times the User Unit Op's Execute() is called.

`Exit Sub`
`EarlyGrave:`
`MsgBox "Execute Error"`	

`End Sub`	Signifies the end of the initialization subroutine. This line does not need to be added.

2. When you are finished entering the code, activate the view by selecting the 'compressed' stream as the Feed on the **Connections** page of the **Design** tab.
3. Go to the **Variables** page to ensure that the **LinkStream** stream name is also 'compressed'.

The Unit Op will not appear 'solved' on the flowsheet, even though it is. This is because UniSim Design expects it to have a fully defined product stream.