Process Simulation Fundamentals

Process Modeling using UniSim® Design

PDS-4526

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Module Index

1. Getting Started

Workshop

The Getting Started module introduces you to some of the basic concepts necessary for creating simulations in UniSim Design. You will use UniSim Design to define three gas streams to be used as feeds to a gas plant. In addition, you will learn how to determine properties of these streams by using the Phase Envelope and the Property Table utilities.

Learning Objectives

- Define a fluid package (property package, components, hypotheticals)
- Add streams
- Understand flash calculations
- Attach stream utilities
- Customize the Workbook

Simulation Basis Manager

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

There are four key advantages to this approach:

- All associated information is defined in a single location, allowing for easy creation and modification of the data.
- Fluid packages can be saved as completely defined entities for use in any simulation.
- Component lists can be saved separately from the Fluid Packages as completely defined entities for use in any simulation.
- Multiple Fluid Packages can be used in the same simulation, however, are all defined inside the common Basis Manager.

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

The first tab of the Simulation Basis Manager allows for the creation of component lists which are independent from fluid packages but can be associated with the individual fluid packages in the case.

There are a number of buttons available to manage the component list(s) used in your case:

Figure 1
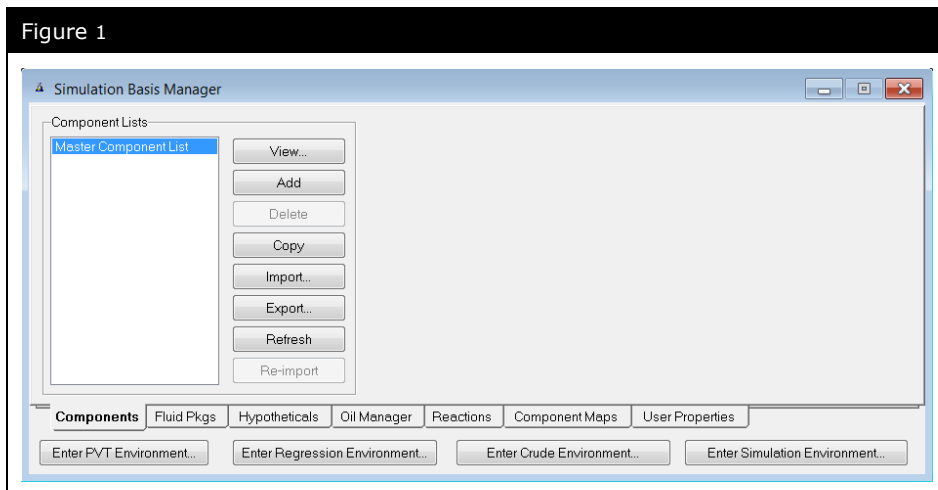
Button	Description
View	Allows you to access the property view for the selected Component List.
Add	Allows you to create a Component List. Note: Component Lists can be added via the Fluid Package property view.
Delete	Removes the selected Component List from the simulation.
Copy	Makes a copy of the selected Component List.
Import	Allows you to import a predefined Component List from disk. Component Lists have the file extension (**.cml**).
Export	Allows you to export the selected Component List to disk. The exported Component List can be retrieved into another case, by using the Import function.
Refresh	Updates the pure component properties from the database.
Re-import	Allows you to re-import a cml file.

Inside the Current Fluid Packages group, there are a number of buttons:

Figure 2
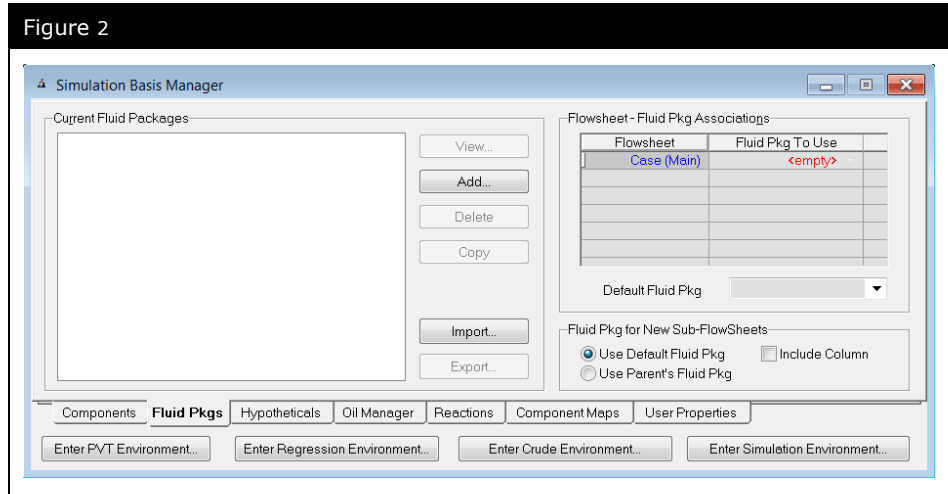
Button	Description
View	This is only active when a Fluid Package exists in the case. It allows you to view the property view for the selected Fluid Package.
Add	Allows you to create and install a Fluid Package in the simulation.
Delete	Removes the selected Fluid Package from the simulation.
Copy	Makes a copy of the selected Fluid Package. Everything is identical in the copied version except the name. This is useful for modifying Fluid Packages.
Import	Allows you to import a predefined Fluid Package from disk. Fluid Packages have the file extension (**.fpk**).
Export	Allows you to export the selected Fluid Package to a disk. The exported Fluid Package can be retrieved into another case by using the Import function.

Defining the Simulation Basis

Add a Property Package

New Case icon

1. Start a new case by selecting the **New Case** icon.
2. Go to the **Fluid Pkgs** tab and create a fluid package by clicking the **Add** button.

3. Scroll down the list and select the **Peng-Robinson** Equation of State model.

You can select the "EOSs" radio button in the Filter box, and then select Peng-Robinson; however, it is not necessary to select EOSs after you have selected Peng-Robinson.

Figure 3
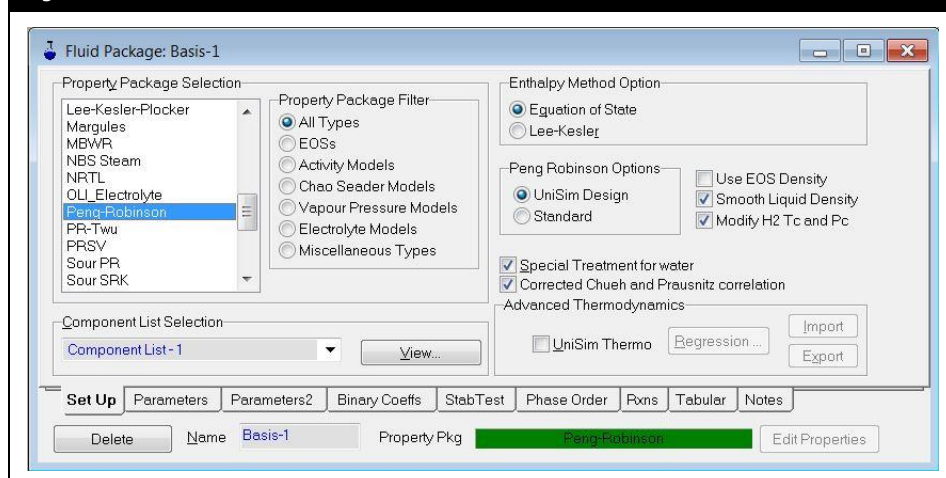
4. Change the Name from the default Basis-1 to **GasPlant** using the **Name** input box at the bottom of the window.
5. Click the **View** button in the Component List Selection section of the **Set Up** tab. This will allow you to add components to the Component List that is now associated with the GasPlant fluid package.

Add Components

You can select components for your simulation using several methods.

You can add a range of components by highlighting the entire range and clicking the Add Pure button.

Standard Windows list conventions (Shift = Select Range, Ctrl = Multi-Select) also work.

To use…	Do this…

Component List	1. Using the scroll bar for the main component list, scroll through the list until you find the desired component.
	2. To add the component, either:
	  • Press the ENTER key.
	  • Click the **Add Pure** button.
	  • Double-click on the component to add it to your simulation.

Match Cell	1. Select one of the three name formats, SimName, Full Name/Synonym, or Formula by selecting the corresponding radio button.
	2. Click in the Match input field and enter the name of the component. As you start to type, the list will change to match what you have entered.
	3. Once the desired component is highlighted, either:
	  • Click the ENTER key.
	  • Click the **Add Pure** button.
	  • Double-click on the component to add it to your simulation.

Filter	1. Ensure the Match cell is empty, and click the **View Filter** button. 2. Select the Use Filter checkbox to display the various family filters. 3. Select the desired family (e.g. Hydrocarbons) from the list of Family Filters to display only that type of component. 4. Use either of the two previous methods to then select the desired component.

6. Select the following library components, using one of the methods described above:

|	
• Nitrogen	• i-Butane
• H2S	• n-Butane
• CO2	• i-Pentane
• Methane	• n-Pentane
• Ethane	• n-Hexane
• Propane	• H2O

Figure 4
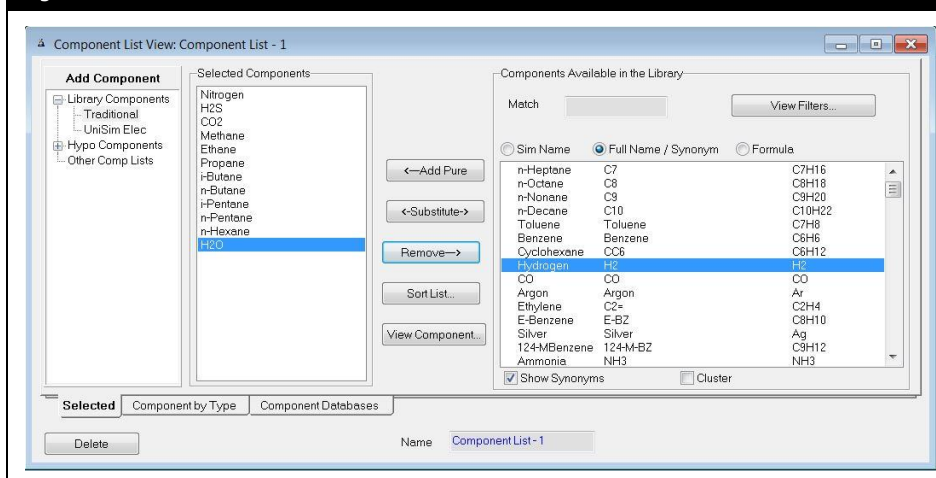
7. Click on the **Hypo Components\Traditional** item in the **Add Component** box.

Figure 5

When you click the **Quick Create a Hypo Component** button, UniSim Design adds a hydrocarbon class hypo by default.

If you want to add a hypo from another class, click the **Hypo Manager** button and then in the view that appears, click the **View Group** button. This will open the Tabular Hypo Group input window, where you can add non-hydrocarbon class hypotheticals.
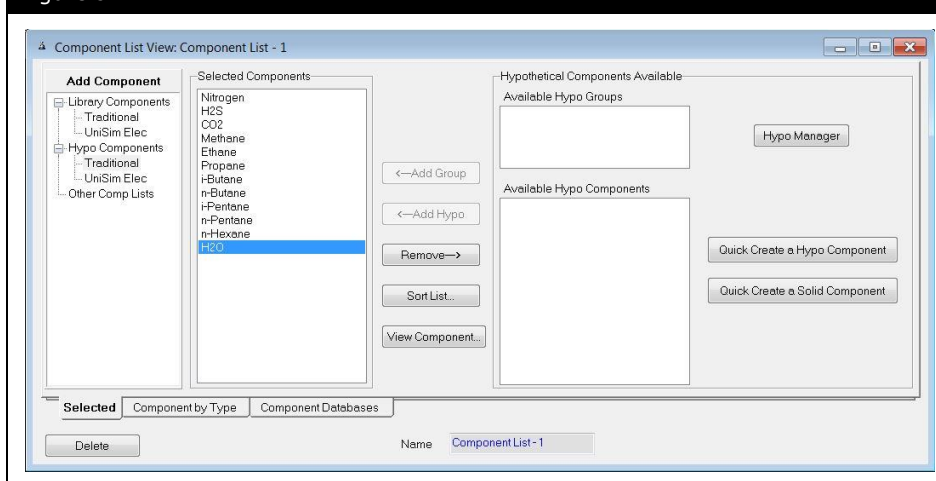
8. Click on the **Quick Create a Hypo Component** button to create a hypothetical component.

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

9. In the hypo component view, click on the **ID** tab and in the Component Name cell type **C7+**.

Figure 6

UniSim Design always places an '*****' after a hypo name so it can be distinguished from library components.

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

10. Click on the **Critical** tab. The only property supplied by the lab for the C7+ component is the Normal Boiling Pt; enter a value of **110°C (230°F)**.

11. Click the **Est Unknown Props** button to estimate all the other properties and fully define the hypothetical component.

Figure 7

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

12. When the hypo component has been defined, return to the component list by closing the hypo component C7+* view.

13. Add the hypo component to the Selected Components list by selecting it in the Available Hypo Components list and then clicking the **Add Hypo** button.

Figure 8

When a component is added to the Selected Components list it appears above the currently selected component.

You can use the **Sort List** button to order the Component List.

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

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

You have now finished defining the fluid package. You can view the Peng-Robinson binary coefficients for your selected components by selecting the **Binary Coeffs** tab on the **Fluid Package** tab.

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

Exporting Fluid Packages

UniSim Design allows you to export fluid packages for use in other simulations. This functionality allows you to create a single common fluid package which you may then use in multiple cases.

14. On the **Fluid Pkgs** tab, highlight the **GasPlant** fluid package.

Figure 9
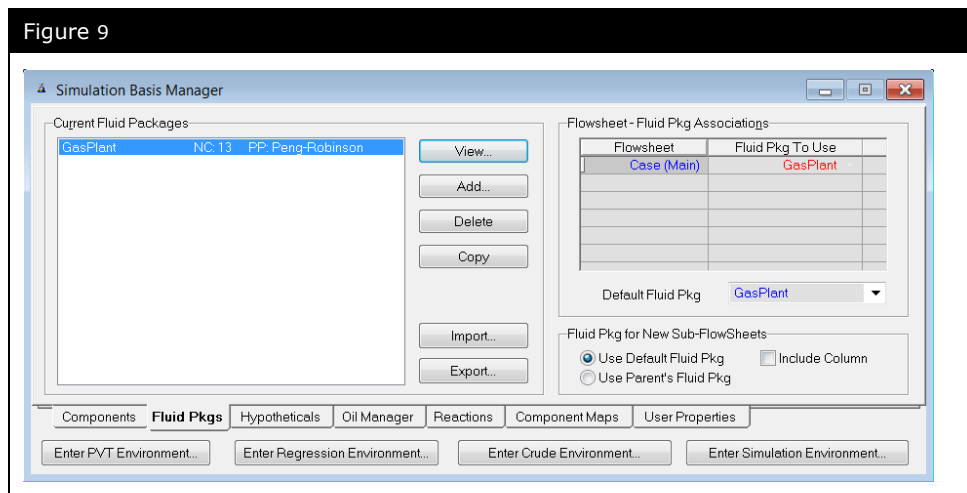
15. Click the **Export** button.
16. Enter a unique name (**4526.01.GasPlant.fpk**) for the fluid package and click the **Save** button.

Figure 10

UniSim Design will automatically add the file extension **.fpk** when it saves your fluid package.

The file is automatically saved to the **\Paks** folder of the UniSim Design folder in My Documents.

Enter Simulation Environment icon
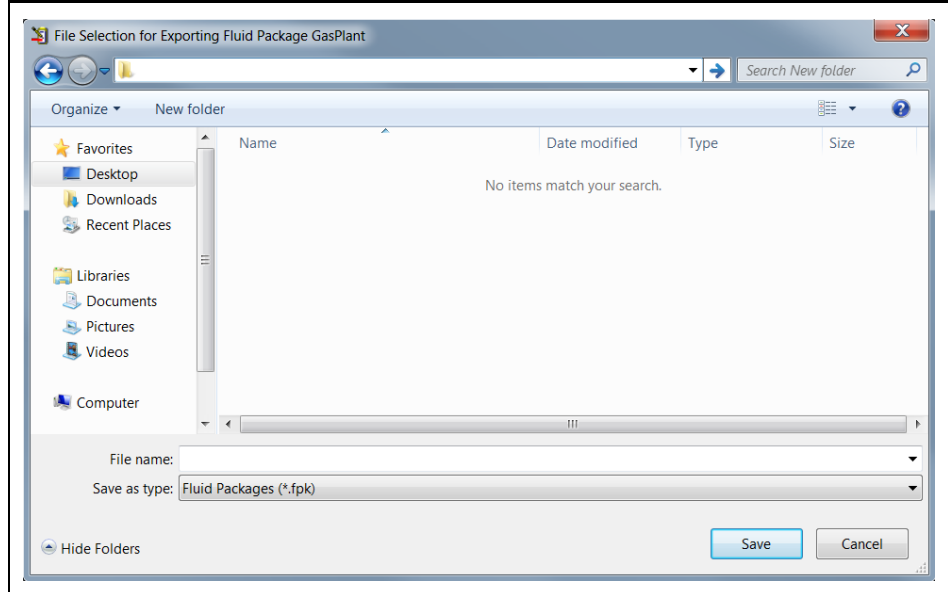
Now that the fluid package has been defined, you can start building the simulation. Click the **Enter Simulation Environment** button on the Simulation Basis Manager window to begin building the simulation.

Basis Environment icon

You can use the **Ctrl B** hot key to re-enter the Simulation Basis Manager at any point or click the Basis Environment icon from the tool bar.

Building the Simulation

When you build the simulation, you will:

- Select a unit set
- Add streams, and specify them
- Attach utilities

Select a Unit Set

In UniSim Design, it is possible to change the unit set used to display its different variables.

1. From the **Tools** menu, choose **Preferences**.
2. Click on the **Variables** tab.

Figure 11

3. Select the **SI** unit set.
4. Close this view to return to the simulation.

Adding Streams

In UniSim Design, there are two types of streams, Material and Energy. **Material streams** have a composition and parameters such as temperature, pressure, and flow rates. They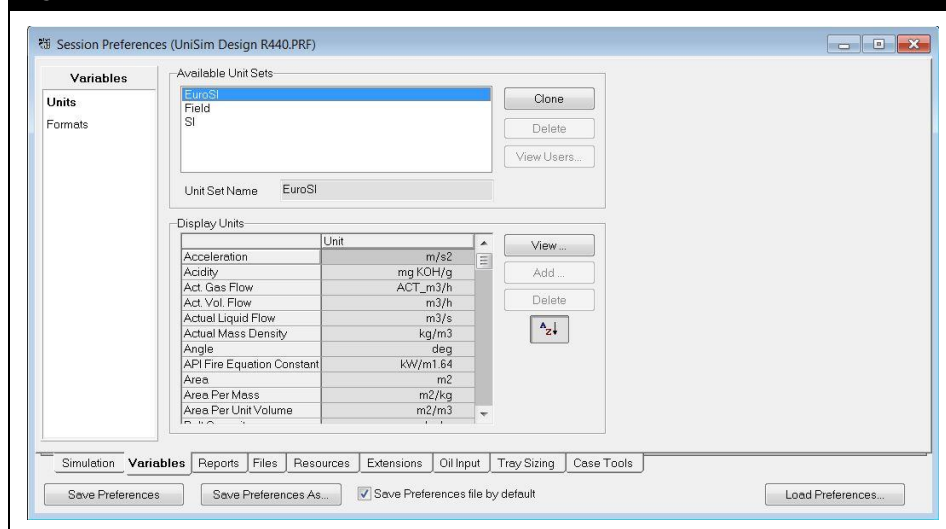 are used to represent process streams. **Energy streams** have only one parameter: heat flow. They are used to represent the duty supplied to or produced by a unit operation.

There are a variety of ways to add streams in UniSim Design.

To use this…	Do this…
Menu Bar	• From the **Flowsheet** menu select **Add Stream**. or • Press the **F11** Hot Key. The Stream property view opens.
Workbook	Open the Workbook and go to the **Streams** tab. Type a stream name into the ****New**** cell.
Object Palette	From the **Flowsheet** menu, select **Open Object Palette** or press **F4** to open the Object Palette. Double-click on the stream icon.

In this case, you will add three streams to represent three different gas wells. Each stream will be added using a different method of installation.

Adding a Stream from the Menu Bar

To add a stream using the **F11** hot key:

1. Press **F11**. The stream property view appears. If the stream property view is not displayed, double-click on the newly created stream (from the PFD) to bring up the property view.

Figure 12
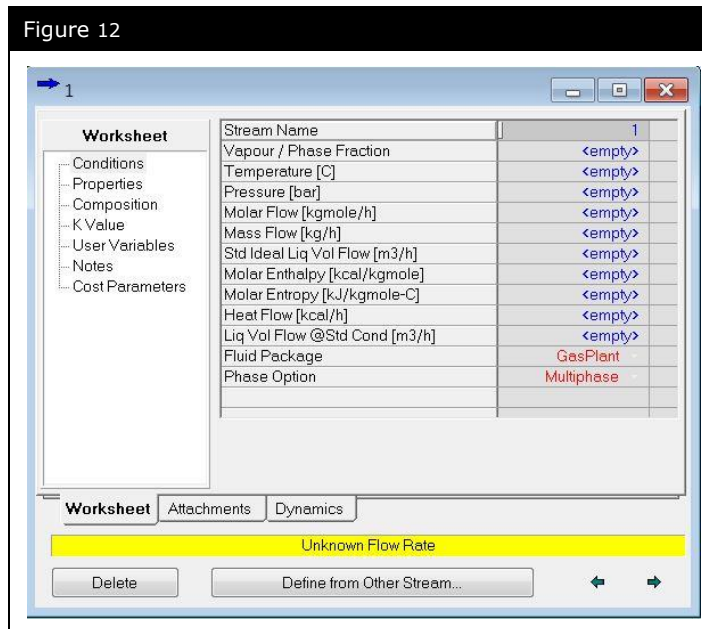
2. Highlight the Stream Name cell. Change the stream name by typing in a new name: **GasWell 1** and then press **ENTER.**

Entering Stream Compositions

Stream compositions are set via the **Input Composition for Stream** window but there are two different ways to access it.

On this page...	Do this...
Conditions	• Double-click on the Molar Flow cell to enter mole fractions. or • Double-click on the Mass Flow cell to enter mass fractions. or • Double-click on the Std Ideal Liquid Volume Flow cell to enter liquid volume fractions. The Input Composition for Stream view appears.
Composition	Click the **Edit** button. The Input Composition for Stream view appears.

3. If the **Input Composition for Stream** view is not already open, double-click on the Molar Flow cell.

Figure 13

The **Normalize** button sets any **<empty>** cells to 0 and adjusts the entered component fractions so that they sum to 1.

The **Equalize Composition** button sets all compositions to 1.

4. Make sure the **Mole Fractions** radio button is set and enter the following compositions:

For this component...	Enter this mole fraction...
Nitrogen	0.0002
H2S	0.0405
CO2	0.0151
Methane	0.7250
Ethane	0.0815
Propane	0.0455
i-Butane	0.0150
n-Butane	0.0180
i-Pentane	0.0120
n-Pentane	0.0130
n-Hexane	0.0090
C7+*	0.0252
H2O	0.0000

Take care when closing the **Input Composition for Stream** view. Changes are only saved when **OK** is pressed. Any non-normalized compositions are automatically normalized when **OK** is pressed.

5. Click the **OK** button when all the mole fractions have been entered

6. Close the Stream property view.

Adding a Stream from the Workbook

Workbook icon

To open the Workbook, click the **Workbook** icon on the tool bar.

1. Enter the stream name, **GasWell 2** in the ****New**** cell.

2. Enter the following Molar compositions:

For this component...	Enter this mole fraction...
Nitrogen	0.0025
H2S	0.0237
CO2	0.0048
Methane	0.6800
Ethane	0.1920
Propane	0.0710
i-Butane	0.0115
n-Butane	0.0085
i-Pentane	0.0036
n-Pentane	0.0021
n-Hexane	0.0003
C7+*	0.0000
H2O	0.0000

3. Click the **OK** button to close the **Input Composition for Stream** view.

Adding a Stream from the Object Palette

Material Stream icon
(Blue)

1. If the Object Palette is not open on the Desktop, press **F4** to open it.

2. Double-click on the **Material Stream** icon. A new stream is added to the flowsheet. Double-click on the new stream to access the Stream property view.

3. Change the name of the stream to **GasWell 3**.

4. Double-click on Molar Flow.

5. Enter the following stream compositions:

For this component...	Enter this mole fraction...
Nitrogen	0.0050
H2S	0.0141
CO2	0.0205
Methane	0.5664
Ethane	0.2545
Propane	0.0145
i-Butane	0.0041
n-Butane	0.0075
i-Pentane	0.0038
n-Pentane	0.0037
n-Hexane	0.0060
C7+*	0.0090
H2O	0.0909

4. Click **OK** to close the **Input Composition for Stream** view.

You can use one of several different methods to save a case in UniSim Design:

Save Case icon

- From the **File** menu, select **Save** to save your case with the same name.
- From the **File** menu, select **Save As** to save your case in a different location or with a different name.
- Click the **Save Case** icon on the tool bar to save your case with the same name.

5. Click the **Save Case** icon, since this case doesn't yet have a file name, enter one (For example 4526.01.GettingStarted.usc)

Save your case often to avoid the possibility of losing information.

Save your case!

Changing Units for a Specification

To change the units for a specification, simply type the numerical value of the specification and press the space bar, or click on the unit drop-down list. Choose the units for the value you are providing. UniSim Design will convert the units back to the default units.

You can scroll through the unit list by starting to type the units, by using the arrow keys, or by using the scroll bar.

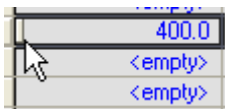To edit an existing value press F2 or use the small vertical bar to the left of the cell.

Figure 14

Flash Calculations

Only two of these five stream parameters (Vapour Fraction, Temperature, Pressure, Enthalpy and Entropy) can be supplied.

UniSim Design can perform several types of flash calculations on streams. The most common types are **Pressure-Temperature (P-T)**, **Vapour Fraction-Pressure (Vf-P)**, and **Vapour Fraction-Temperature (Vf-T)**. Once the composition of the stream and two of either, temperature, pressure or vapour fraction, are known, UniSim Design performs a flash calculation on the stream, calculating the other parameters.

With the flash capabilities of UniSim Design, it is possible to perform dew and bubble point calculations. By specifying a vapour fraction of 1.0 and either the pressure or temperature of the stream, UniSim Design will calculate the dew point temperature or pressure. To calculate the bubble point temperature or pressure, a vapour fraction of 0.0 and either pressure or temperature must be entered.

Perform a P-T flash calculation on the stream GasWell 2. Set the pressure to 7500 kPa and the temperature to 10°C. What is the vapour fraction?

_____

Perform a dew point calculation on the stream GasWell 2. Set the pressure to 7500 kPa. What is the dew point temperature?

_____

Perform a bubble point calculation on the stream GasWell 2. Set the pressure to 7500 kPa. What is the bubble point temperature?

_____

Attaching Utilities

The utilities available in UniSim Design are a set of useful tools that interact with your process, providing additional information or analysis of streams or operations. Once installed, the utility becomes part of the flowsheet, automatically recalculating when conditions change in the stream or operation to which it is attached.

As with the majority of objects in UniSim Design, there are a number of ways to attach utilities to streams:

To use the...	Do this...
Menu Bar	• From the **Tools** menu, select **Utilities**. or • Press **CTRL U**. The **Available Utilities** view appears.
Stream Property View	1. Open the Stream property view. 2. On the **Attachments** tab, click on the **Utilities** page. 3. Click the **Create** button. The **Available Utilities** view appears.

Next, you will add a utility using each method of installation.

Adding a Utility from the Stream Property View

By default the phase envelope is calculated on a dry basis (any water is ignored).

The **Envelope Utility** (in the **Available Utilities** list) allows you to examine relationships between selected parameters for any stream of known composition, including streams with only one component. Vapour-Liquid Envelopes may be plotted for the following variables:

- Pressure - Temperature
- Pressure - Volume
- Pressure - Enthalpy
- Pressure - Entropy
- Temperature - Volume
- Temperature - Enthalpy
- Temperature - Entropy

An Envelope utility will be added to the stream **GasWell 2** from the Stream property view.

1. Open the Stream property view for **GasWell 2** by double-clicking on the stream in either the Workbook or the PFD.

2. On the **Attachments** tab, click the **Utilities** page.

Figure 15
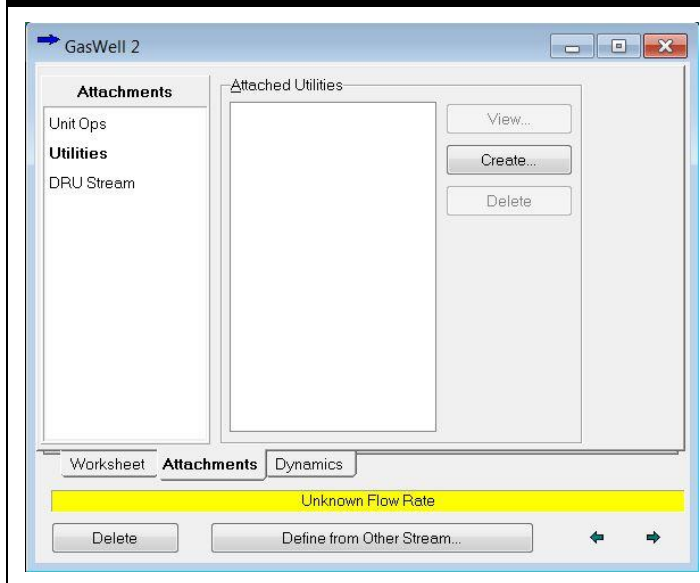
3. Click the **Create** button. The **Available Utilities** view appears.

Figure 16
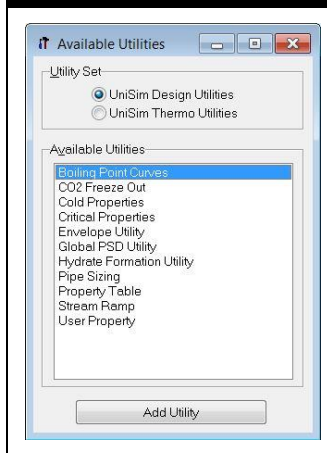
4. Select **Envelope Utility**. Click the **Add Utility** button. The Envelope Utility view appears.

5. The **Design** tab shows the critical and maxima values for the envelope.

What are the critical temperature and pressure for the stream GasWell 2?

*Tc*_____

*Pc*_____

6. Switch to the **Performance** tab to view the phase envelope.

Figure 17
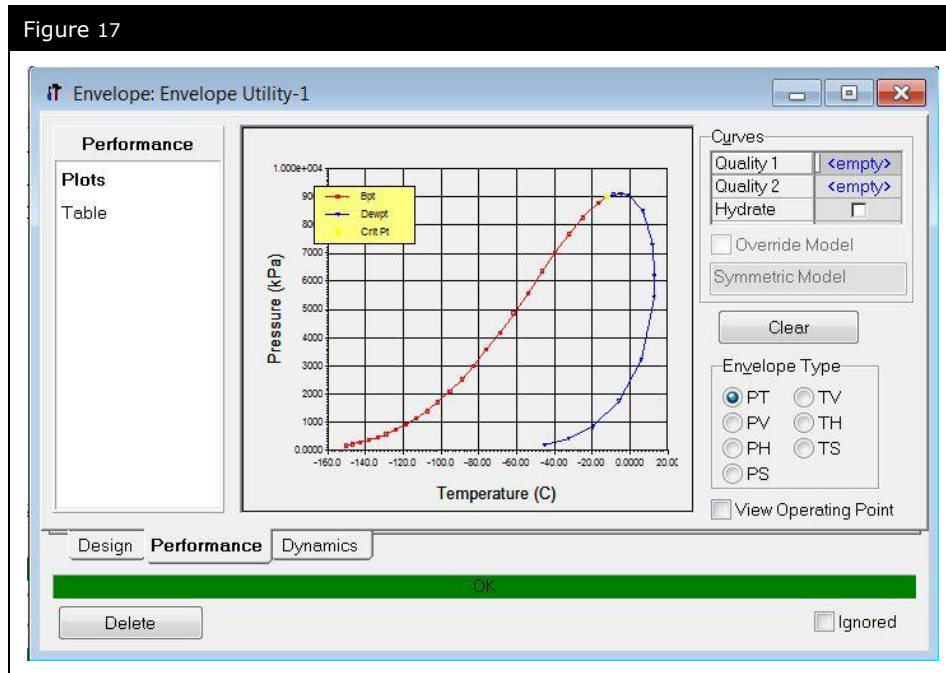
Numerical values can be copied from UniSim Design to Microsoft Excel using the copy command, **Ctrl+C**, in UniSim Design, and then the paste command, **Ctrl+V**, in Excel.

7. Click the **Table** page to view envelope data in tabular format.

Adding a Utility from the Menu Bar

The **Property Table Utility** allows you to examine property trends over a range of conditions in both tabular and graphical formats. The utility calculates dependent variables for user specified independent variable ranges or values.

A Property Table utility will be added to the stream **Gas Well 2**.

1. From the **Tools** menu select **Utilities**, or press **CTRL U**. The Available Utilities view appears.

2. Select **Property Table**.

3. Click the **Add Utility** button. The Property Table view appears.

Figure 18
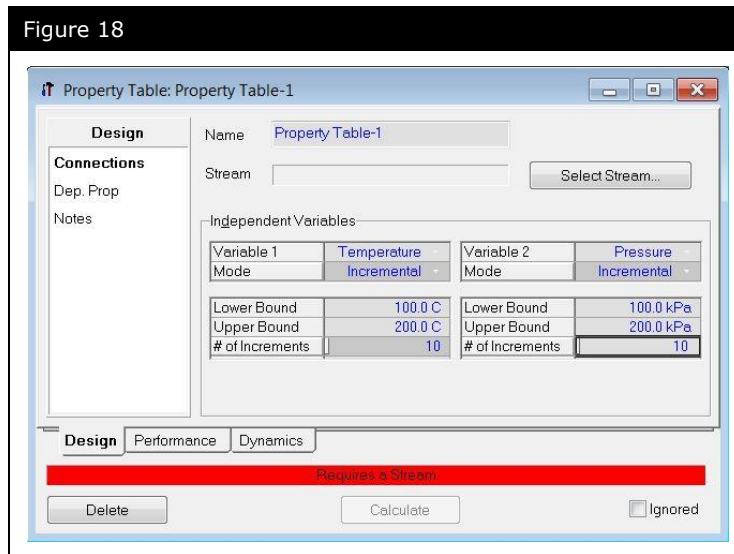
4. Click the **Select Stream** button and select stream **GasWell 2**.

5. Click the **OK** button to return to the Design tab.

6. In the **Independent Variables** section, select **Pressure** as the first **Independent Variable**.

7. Change the mode to **State**, use the drop-down menu bar.

8. In the **State Values** matrix, enter values of **2500, 5000, 7500,** and **9000 kPa**. If you are using field units, the values will be **350, 700, 1050** and **1400 psia**.

9. Choose **Temperature** as the second **Independent Variable**. Ensure the mode is set to **Incremental**.

10. Change the Lower and Upper Bounds to **0°C** (**32°F**) and **100°C** (**212°F**) respectively. Leave **# of Increments** at the default value of **10**.

Figure 19
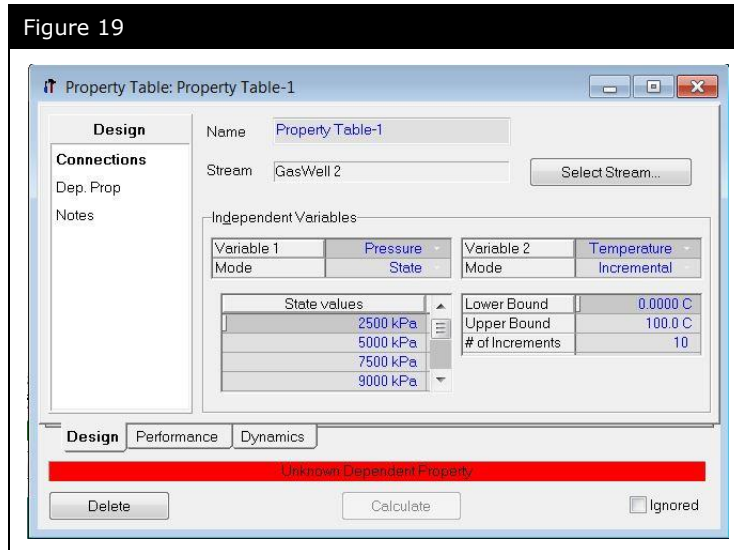
11. On the **Design** tab, click on **Dep. Prop**.

12. On the **Dep. Prop** page, click on the **Add** button.

13. Choose **Mass Density** from the list. Click **OK** to accept.

14. Click on the **Add** button again. Select the **Thermal Conductivity** and click **OK** to accept.

15. Click the **Calculate** button to generate the property table.

16. Examine the property table results in either graphical or tabular format on the **Performance** tab.

Figure 20
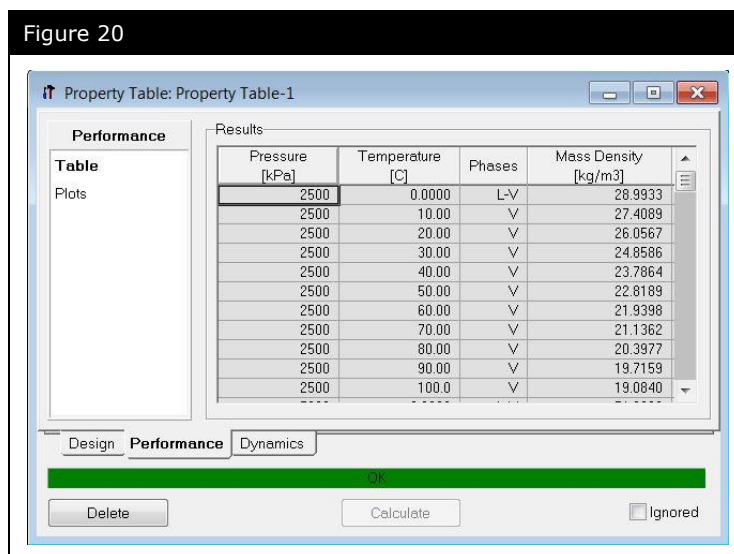
Analyzing the Results

Stream Property View

Within UniSim Design, it is possible to view the properties of the individual phases for any stream.

1. Open the Stream property view for **GasWell 3** by double-clicking on **GasWell 3** in the PFD, and view the **Conditions** page.

2. Add Temperature and Pressure values of **-20°C (-4°F)** and **5000 kPa (725 psia).**

3. Move the mouse arrow to the left or right side of the view until the arrow changes to the double-headed resizing arrows.

4. Press and hold the left mouse button and drag the edge of the view until all the phases can be seen as shown below.

Figure 21

Stream Name	GasWell 3	Vapour Phase	Liquid Phase	Aqueous Phase
Vapour / Phase Fraction	0.7013	0.7013	0.2075	0.0912
Temperature [C]	-20.00	-20.00	-20.00	-20.00
Pressure [kPa]	5000	5000	5000	5000
Molar Flow [kgmole/h]	<empty>	<empty>	<empty>	<empty>
Mass Flow [kg/h]	<empty>	<empty>	<empty>	<empty>
Std Ideal Liq Vol Flow [m3/h]	<empty>	<empty>	<empty>	<empty>
Molar Enthalpy [kJ/kgmole]	-1.116e+005	-8.752e+004	-1.147e+005	-2.894e+005
Molar Entropy [kJ/kgmole-C]	132.2	147.5	120.6	41.11
Heat Flow [kJ/h]	<empty>	<empty>	<empty>	<empty>
Liq Vol Flow @Std Cond [m3/h]	<empty>	<empty>	<empty>	<empty>
Fluid Package	GasPlant	GasPlant	GasPlant	GasPlant
Phase Option	Multiphase	Multiphase	Multiphase	Multiphase

Worksheet: Conditions, Properties, Composition, K Value, User Variables, Notes, Cost Parameters

Worksheet | Attachments | Dynamics

Unknown Flow Rate

Delete   Define from Other Stream...

5. Go to the **Properties** page. This page contains more information about the stream properties.

Figure 22

6. Close the worksheet for **GasWell 3**.

Customizing the Workbook

Workbook icon

UniSim Design allows you to customize the Workbook at several different levels. You can add additional pages, change the variables which are displayed on the current pages, or change the format of the values.

In this exercise, a new Workbook tab containing stream properties, Cp/Cv, Heat of Vapourization, and Molar Enthalpy will be added.

1. Open the Workbook by clicking the **Workbook** icon on the tool bar.

2. From the **Workbook** menu, select **Setup**. The **Setup** view appears as shown below.

The Workbook menu only appears when the Workbook window is active. If the PFD window is active it is replaced by the PFD menu.

Figure 23
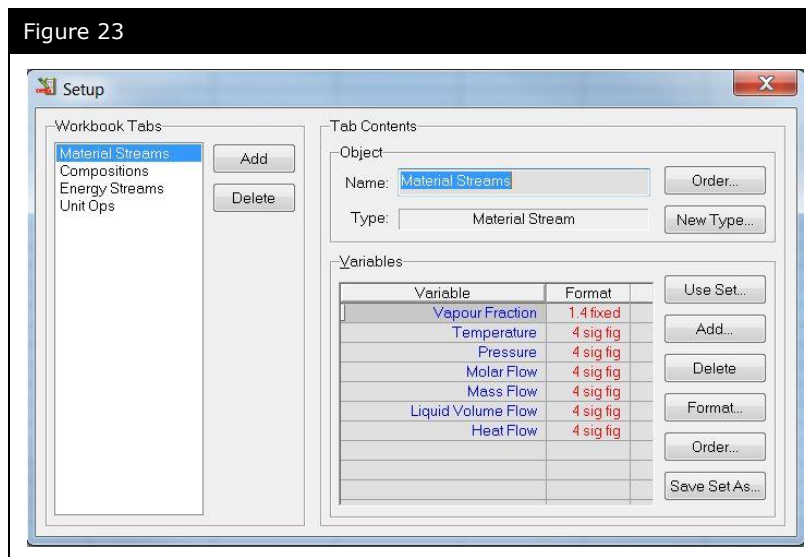
3. Under the **Workbook Tabs** group, click the **Add** button. The **New Object Type** view appears.

Figure 24
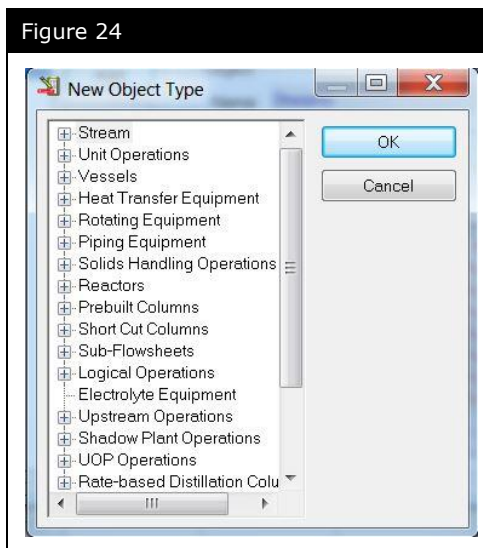
4. Select **Stream** and click **OK**.

5. A new Workbook tab, **Streams**, will be listed in the Workbook Tabs group. Ensure that this new tab is highlighted.

6. Highlight the Name cell and change the name to **Other Props**.

7. In the Variables group, click the **Delete** button until all the default variables are removed.

8. Click the **Add** button to add a new variable to the tab.

9. From the Variable list, select **Cp/Cv** and click **Add**.

10. Repeat step #9 to add **Mass Heat of Vapourization** and **Molar Enthalpy** as shown below and click **Close**

Figure 25
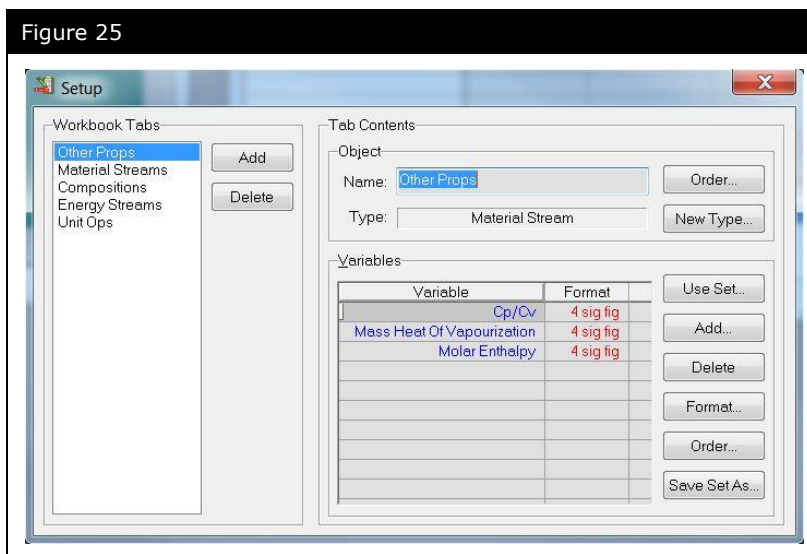
11. When complete close the **Setup** view to return to the Workbook.

12. The Workbook now contains the tab **Other Props** which shows the values of **Cp/Cv**, **Mass Heat of Vapourization**, and **Molar Enthalpy** as shown below.

Figure 26

Printing Stream & Workbook Datasheets

In UniSim Design you have the ability to print Datasheets for streams, operations, and Workbooks.

Printing the Workbook Datasheet

1. Open the Workbook.

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

Workbook icon

Figure 27

The Workbook Datasheet can be used to print a report for all the streams or a subset. To do this:

- If required, use the Order/Hide/Reveal Objects option on the Workbook menu to limit the streams displayed.

- Customize the Workbook to contain all the stream data you want.

- Print the Workbook Datasheet.
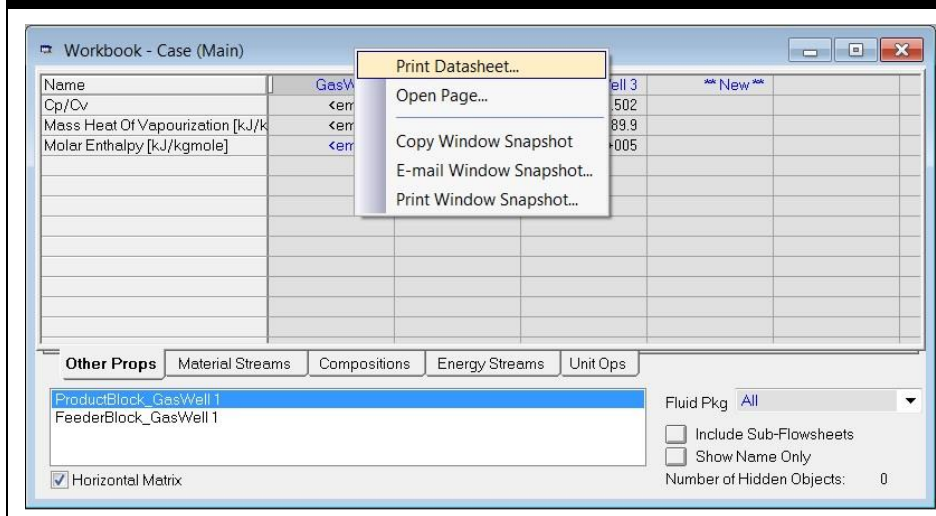
3. Select **Print Datasheet**. The **Select Datablock** view appears.

Figure 28
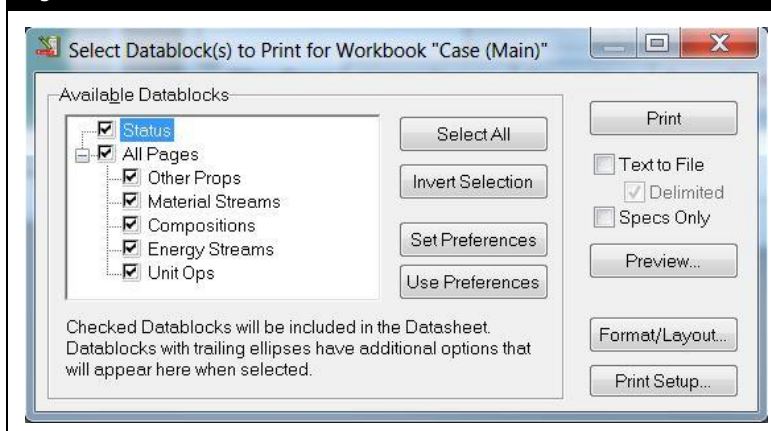
4. From the list, you can choose to print or preview any of the available datasheets.

Printing an Individual Stream Datasheet

To print the datasheet for an individual stream, object inspect the stream property view title bar and follow the same procedure as for the Workbook.

Finishing the Simulation

The final step in this section is to add the stream information necessary for the case to be used in future modules.

Add the following temperature, pressure, and flow rate to the streams:

Stream	Temperature	Pressure	Flow Rate
GasWell 1	40°C (105°F)	4135 kPa (600 psia)	425 kgmole/h (935 lbmole/hr)
GasWell 2	45°C (113°F)	3450 kPa (500 psia)	375 kgmole/h (825 lbmole/hr)
GasWell 3	45°C (113°F)	4175 kPa (605 psia)	575 kgmole/h (1270 lbmole/hr)

Save your case!

Exploring the Simulation

Exercise 1: Phase Behavior & Hydrate Prediction

A. Use the Phase Envelope to find the following values:

Critical Point for GasWell 1.

_____

Cricondenbar (maximum pressure) for GasWell 1.

_____

Bubble Point temperature for GasWell 3 at 6000 kPa.

_____

Dew Point temperature for GasWell 1 at 4000 kPa.

_____

GasWell 1 temperature for 50% quality at 8000 kPa.

_____

Hydrate Formation temperature for GasWell 2 at 7500 kPa.

_____

B Use the Workbook to find the following values:

Bubble Point temperature for GasWell 3 at 6000 kPa.

_____

Dew Point temperature for GasWell 1 at 4000 kPa.

_____

GasWell 1 temperature for 50% quality at 8000 kPa.

_____

C. Use the Hydrate Formation Utility to find the hydrate formation temperature for GasWell 1 and GasWell 2.

Stream	Pressure, kPa (psia)	Hydrate Temperature
GasWell 1	5000 (725)	
GasWell 1	7500 (1090)	
GasWell 2	5000 (725)	
GasWell 2	7500 (1090)	

Challenge

By default the phase envelope utility only performs the flash calculations on a dry basis; it will ignore any water present in the stream.

The envelope utility can perform a calculation including the effect of water if the **UniSim Thermo Three-Phase** option is chosen from combobox at the top right of the **Connections** page.

The composition of **GasWell 3** contains some water. You have been asked to perform a number of Dew and Bubble Point calculations on the stream at various pressures. Knowing that you cannot accurately predict these points on the Phase Envelope (because of the water) you start to do the calculations in the Workbook. After about 30 minutes of doing flashes and writing down the pressure-temperature values, your colleague comes in and tells you the wonders of the Property Table and you are done in about five minutes.

Following your colleague's advice, set up a Property Table to generate a Bubble Point curve and Dew Point curve from 100 to 10000 kPa.

Note: If you make any changes to the temperature and pressure of the streams, be sure to reset them to the values given in the Finishing the Simulation section above before saving your case.

2. Propane Refrigeration Loop

Workshop

Refrigeration systems are commonly found in the natural gas processing industry and in processes related to the petroleum refining, petrochemical, and chemical industries. Refrigeration is used to cool gas to meet a hydrocarbon dew point specification and to produce a marketable liquid.

In this module you will construct, run, analyze, and manipulate a propane refrigeration loop simulation. You will convert the completed simulation to a template, making it available to connect to other simulations.

Learning Objectives

Once you have completed this module, you will be able to:

- Add and connect operations to build a flowsheet
- Use the graphical interface to manipulate flowsheets in UniSim Design
- Understand forward-backward information propagation in UniSim Design
- Convert simulation cases to templates

Prerequisites

Before beginning this module, you need to know how to:

- Define a fluid package
- Define streams
- Navigate the Workbook interface

Process Overview

1		
Temperature	50.00	C
Vapour Fraction	0.0000	
Comp Mole Frac (Propane)	1.0000	

Condenser		
Pressure Drop	35.00	kPa

Chiller		
Duty	1.000e+006	kJ/h
Pressure Drop	7.000	kPa

Compressor	
Adiabatic Efficiency	75

3		
Temperature	-20.00	C
Vapour Fraction	1.0000	
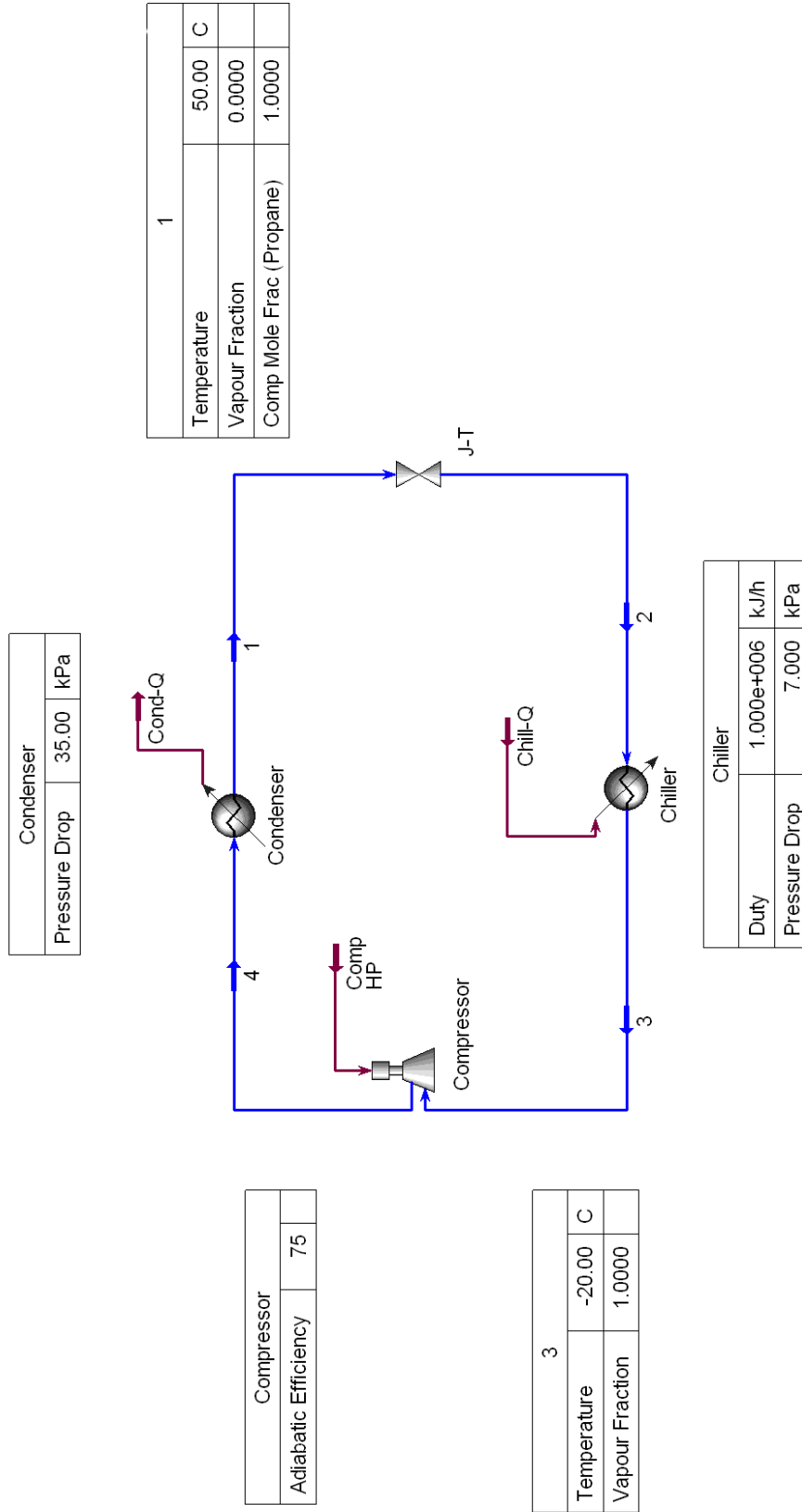
Building the Simulation

The first step in building any simulation is defining the fluid package. A brief recap on how to define a fluid package and install streams is described below. (For a complete description, see the previous module).

Defining the Simulation Basis

1. Create a New Case and add a fluid package.
2. Specify the following property package and component:

On this page...	Select...
Property Package	Peng-Robinson
Components	Propane

Enter Simulation Environment icon

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

Installing a Stream

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

- Press **F11**. The Stream property view appears.

or

- Double-click the Stream icon in the Object Palette.

Defining Necessary Streams

Add a stream with the following values:

In this cell...	Enter...
Name	1
Vapour Fraction	0.0
Temperature	50°C (120°F)
Composition	Propane - 100%

Add a second stream with the following properties:

In this cell...	Enter...
Name	3
Vapour Fraction	1.0
Temperature	-20°C (-4°F)

What is the pressure of Stream 1?

_____

Adding Unit Operations to a Flowsheet

As with streams, there are a variety of ways to add unit operations in UniSim Design:

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

The propane refrigeration loop consists of four operations:

- Valve
- Chiller
- Compressor
- Condenser

In this exercise, you will add each operation using a different method of installation.

Adding a J-T Valve

The J-T Valve is modeled using the Valve operation in UniSim Design. The inlet to the valve comes from the condenser outlet. The condenser outlet is at its bubble point.

The valve will be added using the **F12** hot key.

You can filter the Available Unit Operations list by selecting an appropriate Category. In this case, **Piping Equipment** would filter the list to include the Valve operation.

1. Press **F12**. The **UnitOps** view appears:

Figure 1
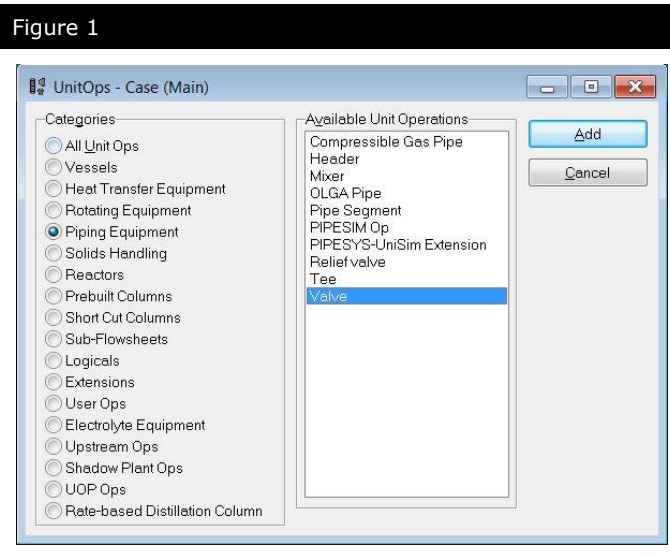
2. Select **Valve** from the **Available Unit Operations** list.
3. Click the **Add** button. The Valve property view appears.
4. On the **Connections** page, supply the inlet and outlet connections as shown below:
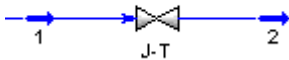
Figure 2

Drop-down lists, such as for the Feed and Product streams, contain lists of available streams which can be connected to the operation.
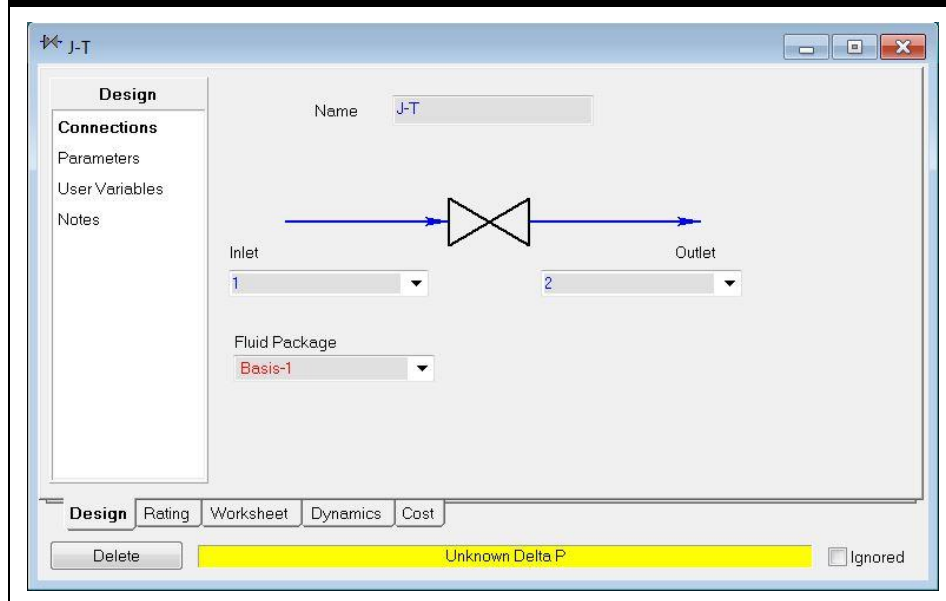
Adding a Chiller

The Chiller operation in the propane loop is modeled in UniSim Design using a Heater operation. The outlet of the Chiller will be at its dew point.

To add a heater:

1. Open the Workbook and click the **Unit Ops** tab.
2. Click the **Add UnitOp** button. The **UnitOps** view appears.
3. Select **Heat Transfer Equipment** from the **Categories** group.
4. Select **Heater** from the **Available Unit Operations** list as shown below.

Figure 3
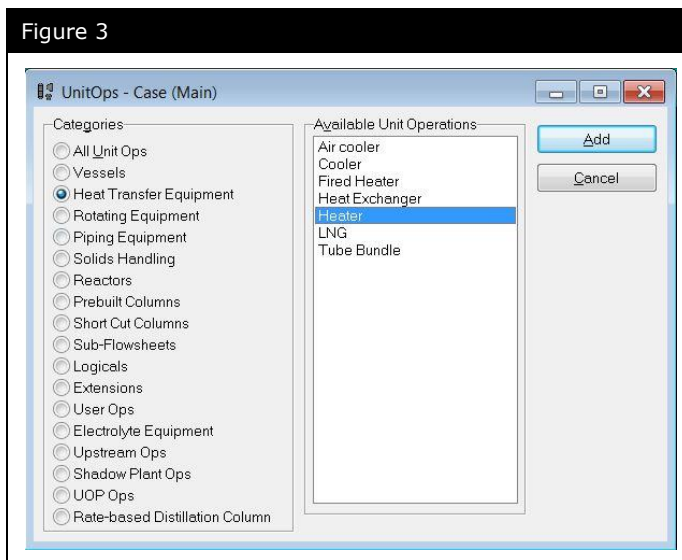
5. Click the **Add** button, or double click on Heater. The Heater property view appears.

6. On the **Connections** page, enter the information as shown below:

Figure 4
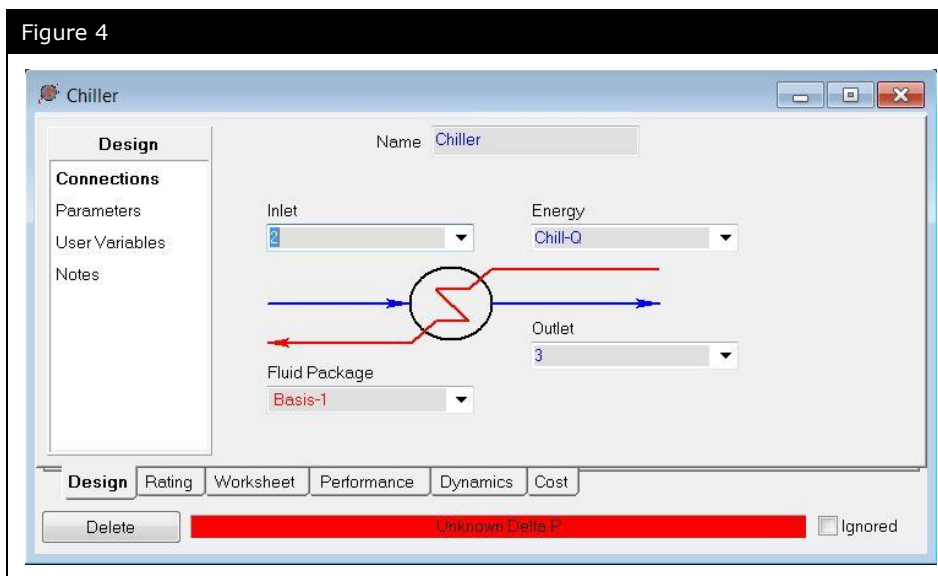
7. Go to the **Parameters** page.

8. Enter a **Delta P** value of **7.0 kPa** (1 psi) and a **Duty** value of **1.00e+006 kJ/h** (1.00e+06 Btu/hr) for the Chiller.

The **Parameters** page will be common to most unit operations and contains parameters such as Delta P, Duty, and Efficiency.

Figure 5
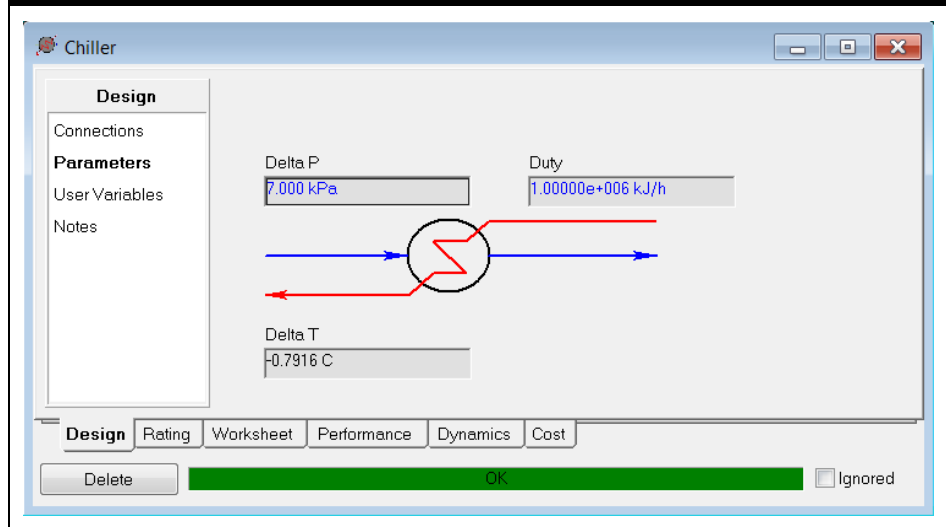
9. Close the property view.

> **What is the molar flow rate of propane?**
> _____
>
> **What is the pressure drop across the J-T valve?**
> _____
>
> **What is the temperature of the valve outlet (stream 2)?**
> _____

Compressor icon

Adding a Compressor

The Compressor operation is used to increase the pressure of an inlet gas stream.

To add a compressor:

1. Press **F4**. The Object Palette appears.

2. Double-click the **Compressor** icon on the Object Palette. The Compressor property view appears.

3. On the **Connections** page, enter the stream information as shown below:
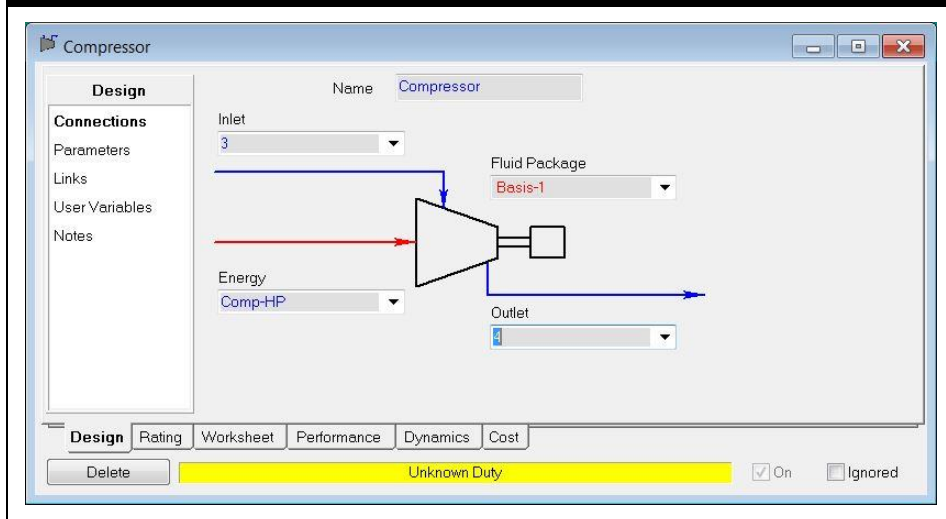
Figure 6

4. On the **Parameters** page, leave the **Adiabatic Efficiency** at its default value of **75%** as shown below:
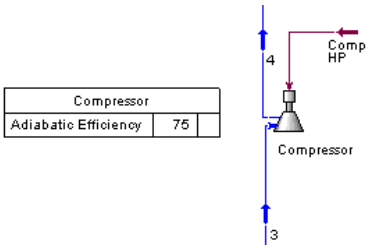
Figure 7
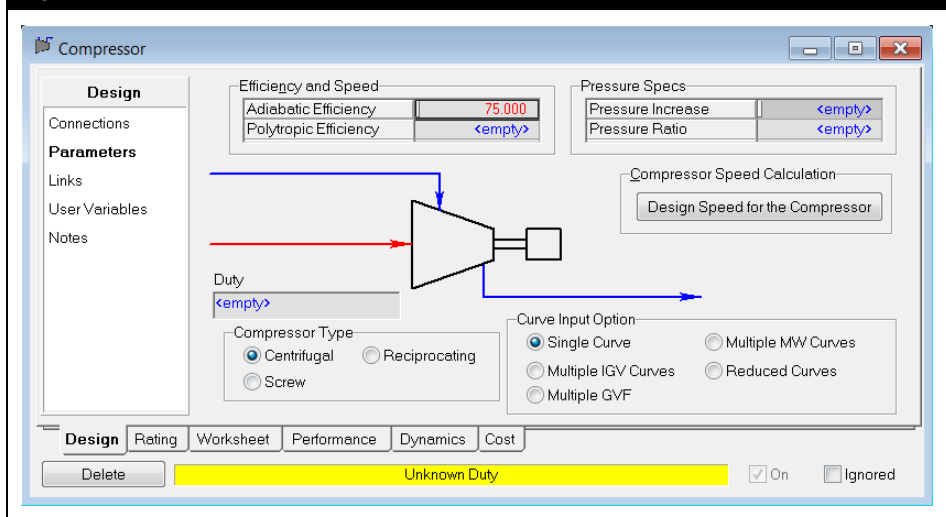
Adding the Condenser

The Condenser operation completes the propane refrigeration loop. It is placed between the Compressor and the Valve and is modeled as a Cooler operation.

Working with a graphical representation, you can build your flowsheet in the PFD using the mouse to install and connect objects. This procedure describes how to install and connect the Cooler using the Object Palette drag 'n' drop technique.

Using Drag 'n' Drop in the PFD

Cooler icon

1. Click the **Cooler** icon on the Object Palette.
2. Move the cursor to the PFD. The cursor will change to a special cursor, with a box and a plus (+) symbol attached to it. The box indicates the size and location of the cooler icon.
3. Click again to "drop" the cooler onto the PFD.

There are two ways to connect the operation to a stream on the PFD:
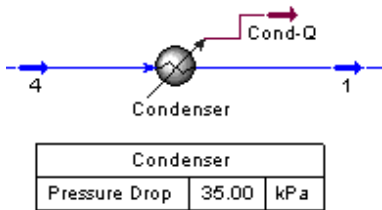
To connect using the...	Do this...
Attach Mode toggle	1. Press the **Attach Mode** toggle button on the PFD button bar.
	2. Place the cursor over the operation. The connection points are highlighted as squares and rectangles. Material stream connections are dark blue, energy stream connections are red.
	3. Move the cursor over the connection you want to make. When over the connection the cursor icon changes to one with a white square, and a pop up message tells you which connection it is.
	4. Press and hold the left mouse button.
	5. Move the cursor to the stream icon you wish to connect, if a connection is allowed a square connection point appears.
	6. Move the cursor over the connection point and release the mouse button.
CTRL key	1. Press and hold the **CTRL** key, notice that the Attach Mode button appears depressed.
	2. Follow the same steps as above
	3. When complete, release the **CTRL** key.

4. From the PFD, connect stream **4** to the Condenser inlet and connect the Condenser outlet to stream **1** using one of the methods in the table above.
5. Add an **Energy Stream**. Change the name to **Cond-Q.**
6. Double-click on the Condenser.
7. On the **Parameters** page, enter a Delta P of **35 kPa** (5 psi).

Figure 8
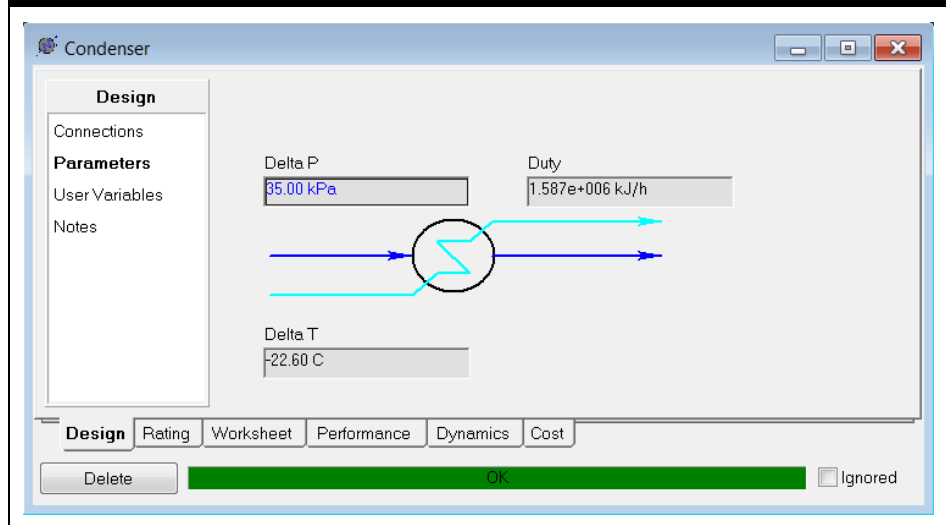
What is the compressor energy in hp?

_____

Hint: Clone a unit set and set the Power to "hp" units.

Save your case!

Undo/Redo/Recent Values

UniSim Design offers an undo/redo facility. It applies in the following circumstances:

- Values entered into object property values (streams/unit operations)
- PFD object moves and resizing

Object Property Views

In any object property view (e.g. a material stream or any unit operation) UniSim Design has an unlimited undo/redo feature.

To use undo/redo use the **Undo** and **Redo** options on the **Edit** menu or the short cut keys **CTRL Z** and **CTRL Y**.
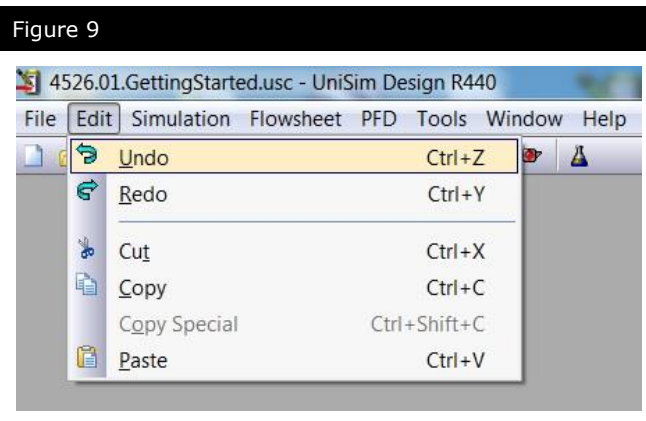
Figure 9

Additionally by right clicking on any specified value a list of all recent entered values can be entered.

Figure 10
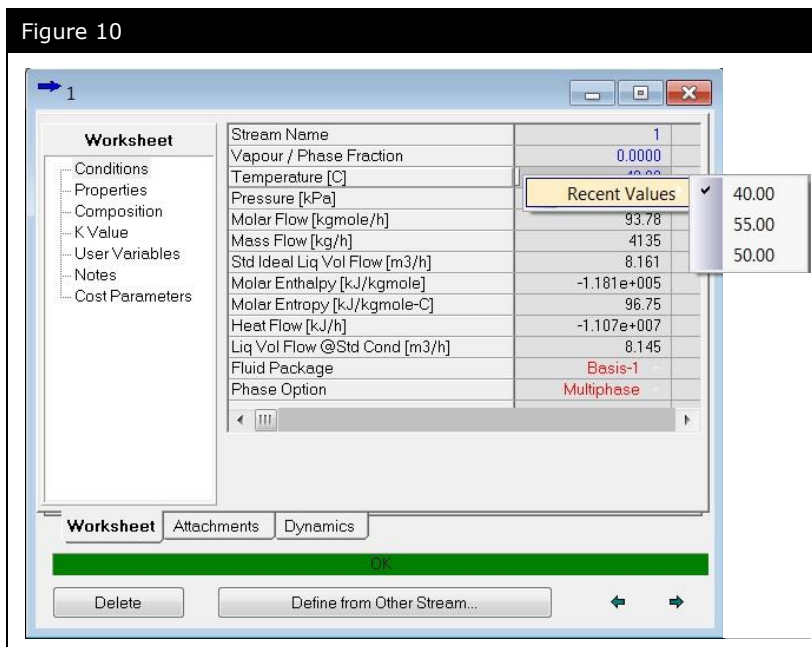
> Note that any undo/redo/recent values information is lost when the object property view is closed. Each time an object property view is opened fresh undo/redo/recent values information is stored.
>
> Note also that using the undo/redo/recent values facility has the same effect as typing the value in the cell; any other parts of the flowsheet that depend on the value will recalculate accordingly.

PFD object moves and resizing

UniSim Design also has an unlimited undo/redo facility for object moves and object resizing on the PFD. This is also accessed by the **Undo** and **Redo** options on the **Edit** menu or the short cut keys **CTRL Z** and **CTRL Y.**

> Note that any undo/redo information is lost when the PFD window is closed. Each time a PFD window is opened fresh undo/redo information is stored.
>
> Note also that you cannot undo object deletion.
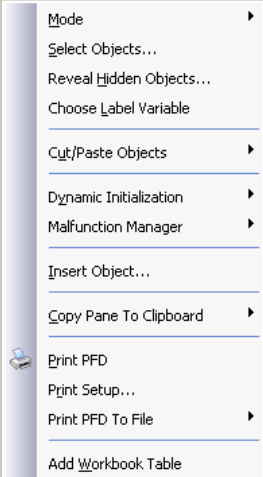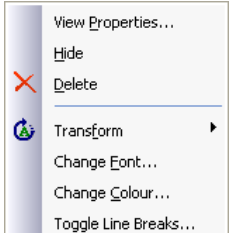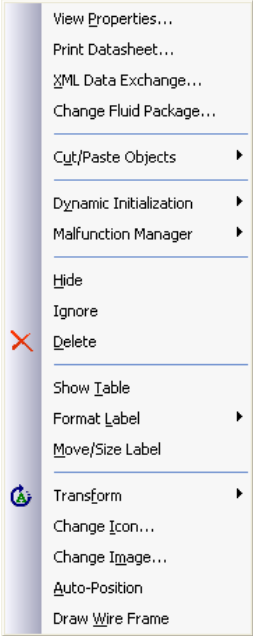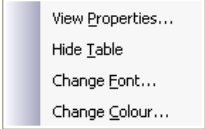
Manipulating the PFD
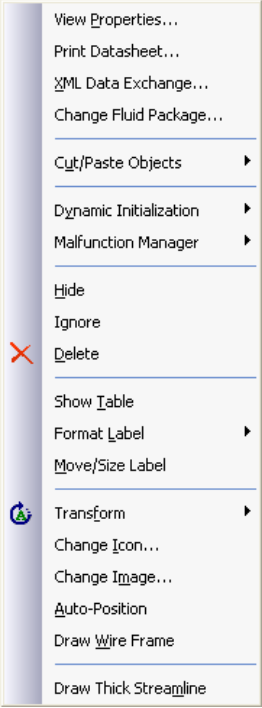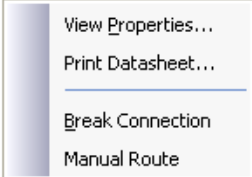
The PFD is designed around using the mouse and/or keyboard. There are a number of instances in which either the mouse or the keyboard can be used to perform the same function. One very important PFD function for which the keyboard cannot be used is object inspection.

You can perform many of the possible tasks and manipulations on the icons in the PFD by using object inspection. Place the mouse arrow over the object you want to inspect and press the right mouse button. An appropriate menu is produced depending upon the object selected (Stream, Streamline, Operation, Column, PFD Table, PFD Background, Text Annotation etc.).

A list of the objects that you can object inspect are shown in the following table with the corresponding menus.

Object...	Object Inspection Menu...
PFD	Mode ▶ Select Objects... Reveal Hidden Objects... Choose Label Variable Cut/Paste Objects ▶ Dynamic Initialization ▶ Malfunction Manager ▶ Insert Object... Copy Pane To Clipboard ▶ Print PFD Print Setup... Print PFD To File ▶ Add Workbook Table
Text Annotations	View Properties... Hide Delete Transform ▶ Change Font... Change Colour... Toggle Line Breaks...

Object...	Object Inspection Menu...
Unit Operations	
Unit Operation Tables	
Workbook Tables	

Object...	Object Inspection Menu...
Streams (Depending on where on the stream you click, either of these two menus will appear. To see the long menu, right-click on the stream icon. To see the short menu, right-click on the stream line).	View Properties... Print Datasheet... XML Data Exchange... Change Fluid Package... Cut/Paste Objects ▶ Dynamic Initialization ▶ Malfunction Manager ▶ Hide Ignore Delete Show Table Format Label ▶ Move/Size Label Transform ▶ Change Icon... Change Image... Auto-Position Draw Wire Frame Draw Thick Streamline View Properties... Print Datasheet... Break Connection Manual Route

Add Text icon

The width of the text box is modified by clicking the **Size Mode** button on the PFD button bar and then clicking on the text box. Click on either white square that appears on the left and right side of the text box and drag to desired width.

Customize the PFD by performing the following:

1. Add the Title: **Propane Refrigeration Loop** by clicking the **Add Text** icon on the PFD tool bar. Move the cursor to an appropriate location on the PFD where the text should be displayed and left-click the mouse button. Type the title text in the **Text Props View** that appears and click **OK**. Modify the title color, font and size from the options available in the Text Annotations menu. **Hint:** right-click on the title to see this menu.

2. Add a Workbook Table for the material streams in the simulation. **Hint:** right click on the PFD background and use the **Add Workbook Table** option.

3. Add a Table for Stream 4. **Hint:** right-click on Stream 4

Note that existing tables can be modified by double clicking on them and making the desired changes.

Save your case!

Saving the Simulation as a Template

A template is a complete flowsheet that has been stored to disk with additional information included so that the flowsheet can be added to another model as a sub-flowsheet operation.

Typically, a template is representative of a plant process module or portion of a process module. The stored template can subsequently be read from disk and efficiently installed as a complete sub-flowsheet operation any number of times into any number of different simulations.

Some of the advantages of using templates are:

- Provides a mechanism by which two or more cases can be linked together
- Employs a different property package than the main case to which it is attached
- Provides a convenient method for breaking large simulations into smaller, easily managed components
- Is created once and can be installed in multiple cases

Before you convert the case to a template, it needs to be made generic so it can be used with gas plants of various flow rates. In this case, the Chiller Duty dictates the flow rate of propane required.

1. Delete the **Chiller Duty** value.
2. From the **Simulation** menu, select **Main Properties**. The Simulation Case view appears as shown below.

Figure 11
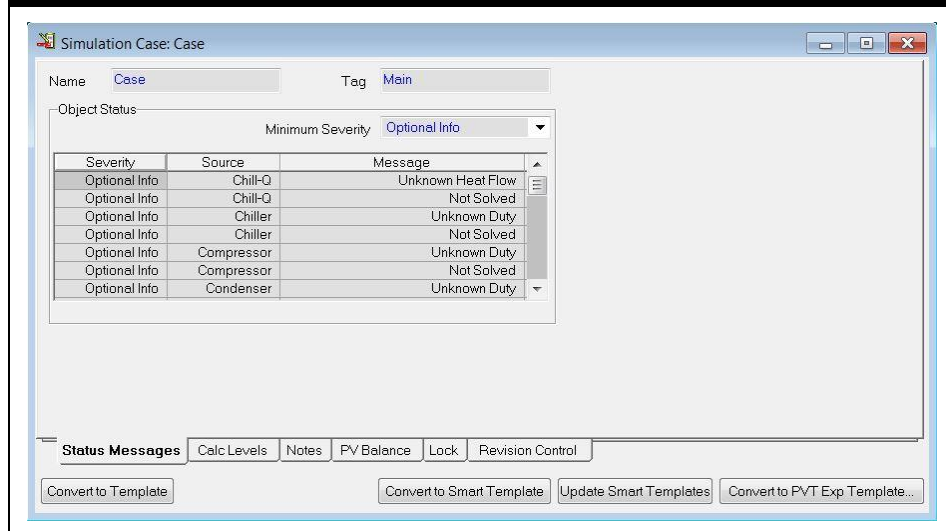
3. Click the **Convert to Template** button.

4. Click **Yes** to convert the simulation case to a template.

5. Answer **No** to the question **"Do you want to save the simulation case?"**.

6. Go to the File menu and **Save** the template as **4526.02.C3Loop.utpl**.

Analyzing the Results

This section describes how to retrieve and print unit operation results.

Printing Datasheets for Unit Operations

In UniSim Design you can print results through:

- The menu bar
- Object inspection of unit operations
- The Report Manager

To set up the printer, select **Printer Setup** from the **File** menu, then select either the **Graphic Printer** or the **Report Printer**. This allows you to set the printer configuration: printer, paper, size, source and orientation.

Printing Using the Menu Bar

Choose one of the following options from the **File** menu:

- **Print**. Lists the available Datasheets for the active unit operation. You can highlight a Datasheet and either preview or print it.

Choosing the **Print** command when the PFD is the active view will print the PFD. There are no datasheets available for the PFD.

Figure 12
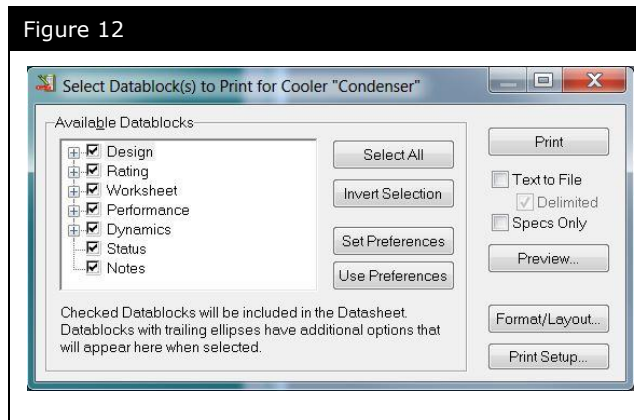
- **Print Window Snapshot**. Prints a bitmap of the active UniSim Design view.

Printing Using Object Inspection

Object inspect the Title Bar of the unit operation property view and select **Print Datasheet**. A list of available Datablocks is displayed for the object.

Printing Using Report Manager

1. Open the **Tools** menu. Select **Reports**. The Report Manager view appears as shown below.
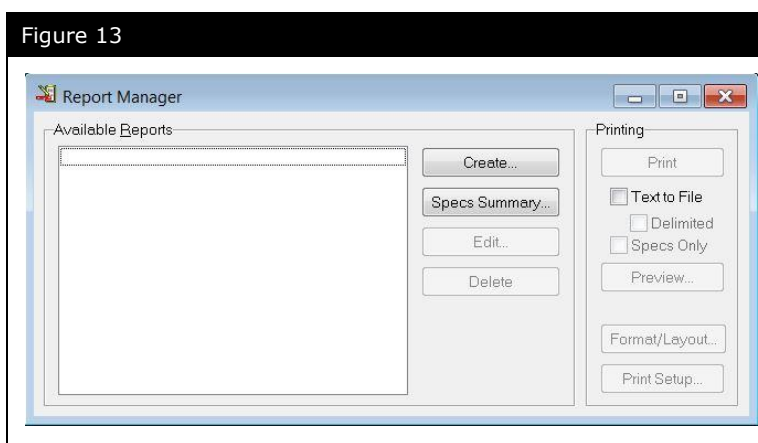
Figure 13

2. Click the **Create** button to add a new report. The Report Builder view appears as shown below.

Figure 14
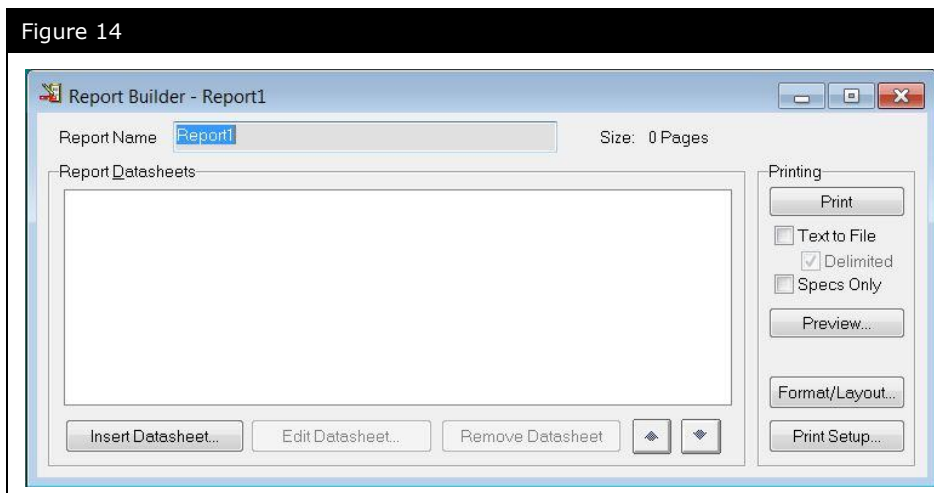
3. Click the **Insert Datasheet** button to add datasheets to your report. You can add single or multiple unit operation Datasheets to a report.

Figure 15
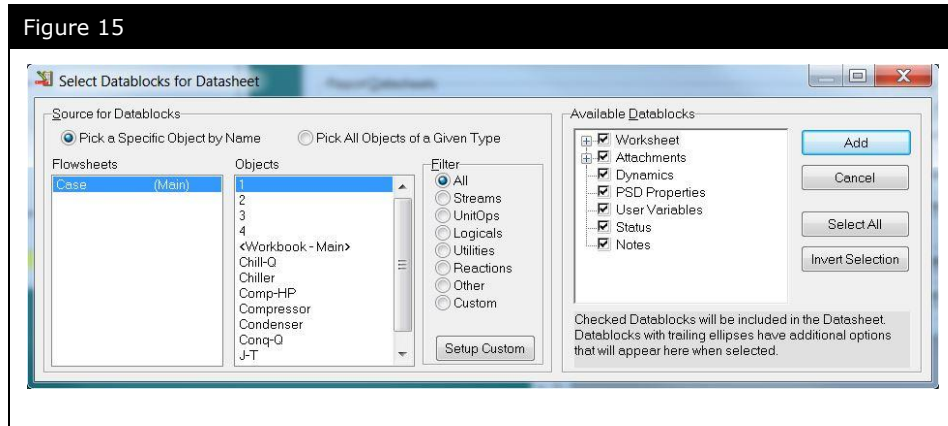
Adding Unit Operation Data to the Workbook

Each WorkBook has a Unit Ops page by default that displays all the unit operations and their connections in the simulation. You can add additional pages for specific unit operations to the WorkBook. For example, you can add a page to the WorkBook that contains only the compressors in the simulation.

Adding a Unit Operation Tab to the WorkBook

1. Open the **Workbook**. Open the **Workbook** menu. Select **Setup**. The Setup view appears.

2. Click the **Add** button in the Workbook Tabs group. The New Object Type view appears.

3. Select **Rotating Equipment** and expand the list. Select **Compressor** as shown.

Clicking on an entry with a "+" sign will open an expanded menu.

Figure 16
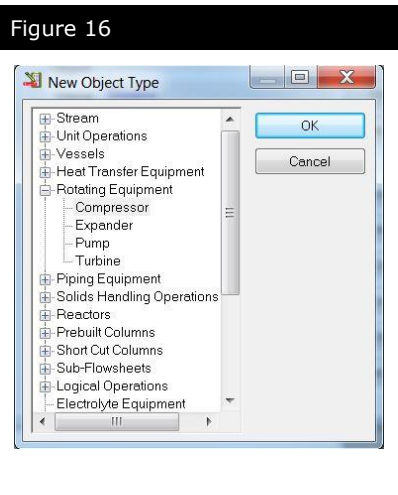
4. Click **OK**. A new page, **Compressors**, containing only compressor information is added to the Workbook.

5. Close this view.

Adding Unit Operation Data to the PFD

For each unit operation, you can display a Property Table on the PFD. The Property Table contains certain default information about the unit operation.

Adding Unit Operation Information to the PFD

Remember you can Object Inspect an object by selecting it and then clicking on it with the right mouse button.

1. Open the PFD.
2. Select the unit operation for which you want to add the Property Table.
3. Object Inspect the unit operation.
4. Click **Show Table**.
5. After the table has been added, you can move it by selecting it and dragging it with the mouse.
6. If you Object Inspect the table, you can change its properties and appearance. You can also specify which variables the table will show.

Advanced Modeling

One of the key design aspects of UniSim Design is how Modular Operations are combined with a Non-Sequential solution algorithm. Not only is information processed as you supply it, but the results of any calculation are automatically propagated throughout the flowsheet, both forwards and backwards. The modular structure of the operations means that they calculate in either direction, using information in an outlet stream to calculate inlet conditions. This design aspect is illustrated using the Propane Refrigeration Loop.

Figure 17
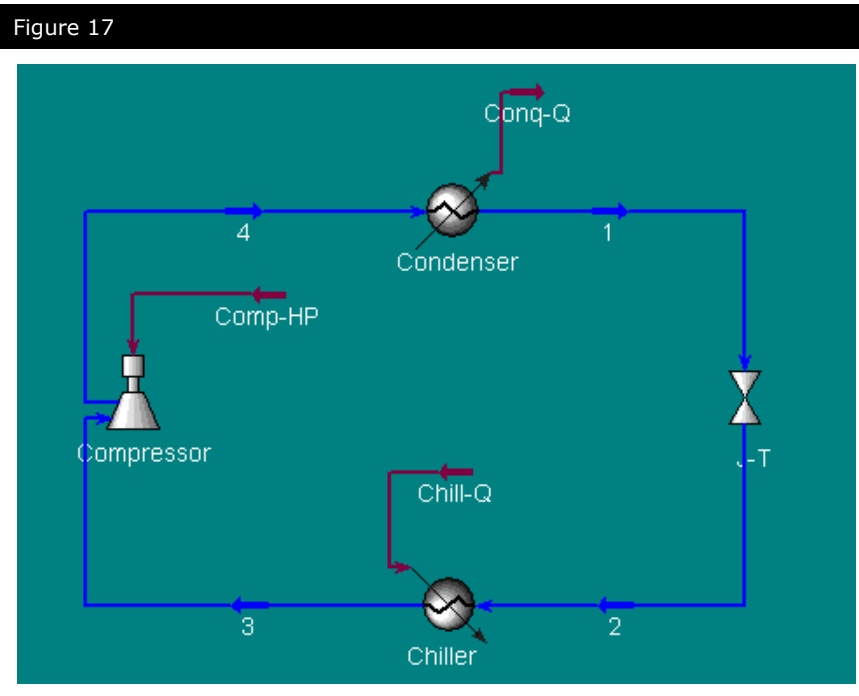
Initially, the only information supplied in the case is the temperature and vapour fraction for streams 1 and 3 and the composition of stream 1. Since the temperature, vapour fraction, and composition of stream 1 are known, UniSim Design will automatically perform a flash calculation and determine the remaining properties (pressure, intensive enthalpy, density, etc.) which are independent of flow.

When streams 1 and 2 are attached to the valve J-T, UniSim Design first determines what information is known in either the input or output stream. It will then assign these values to the other stream. In this case, since no valve pressure drop was specified, only the composition and intensive enthalpy of stream 1 will be passed to stream 2.

By attaching stream 2 and 3 to the heater operation, Chiller, the composition of stream 2 is passed to stream 3 (100% Propane). UniSim Design can now perform a flash calculation on stream 3 and determine the remaining properties which are independent of flow, i.e. pressure, enthalpy, etc.

Using the calculated pressure of stream 3 and the specified pressure drop across the heater, UniSim Design back calculates the pressure of stream 2. Since pressure, composition and intensive enthalpy of stream 2 are now known (the valve is isenthalpic), UniSim Design can calculate the temperature of stream 2.

In addition, UniSim Design uses the specified heater duty and the intensive enthalpy of streams 2 and 3 to calculate the flow rate, which is then passed on to streams 1, 2 and 3.

Next, the Compressor is added to the simulation. Since all of the inlet information is known, the compressor has only 2 degrees of freedom remaining. Parameters such as Efficiency, Duty, or Outlet Pressure can satisfy one degree of freedom. The second degree of freedom comes from the Condenser.

The Condenser connects the Compressor outlet to the Valve inlet (which is completely defined). The user supplies the Condenser pressure drop, and UniSim Design calculates the inlet pressure, which is also the Compressor outlet pressure (the second degree of freedom for the Compressor).

Exploring the Simulation

Use your saved case (not the template) for the following exercises.

Exercise 1: Design vs. Rating Scenarios

In the plant, you are unable to accurately measure or calculate the chiller duty. You do, however, know that the compressor is rated for 250 hp and that it is running at 90% of maximum and 72% efficiency.

> *What is the chiller duty?*
> _____

The Chiller Gas Flow meter has finally been calibrated and you can determine the chiller duty. It has been decided to increase the chiller duty to 1.5 MMBTU/hr.

> *With the compressor running at the same horsepower (225 hp), what is the best chiller outlet temperature you can achieve (and thus maximize cooling for the process) while still running the compressor at a reasonable operating point?*
> _____

Exercise 2: Refrigerant Composition

> **Before starting this exercise return the refrigeration loop to its original configuration: Chiller duty specified (1.00e+006 kJ/h), compressor adiabatic efficiency specified (75%) and power calculated, chiller outlet temperature specified (-20°C).**

Your local propane dealer arrives at your plant selling a 95/5 (mole%) Propane/Ethane blend.

> *What effect, if any, does this new composition have on the refrigeration loop?*
>
> _____

Use the base case for comparison:

	Base Case: 100% Propane	New Case: 5% Ethane, 95% Propane
Flow, kgmole/h		
Condenser Q, kJ/h		
Compressor Q, hp		

Challenge: Adding an Economizer

Create a two stage refrigeration loop by adding an Economizer.

> ***What is the net compression in hp?***
> _____

Figure 18
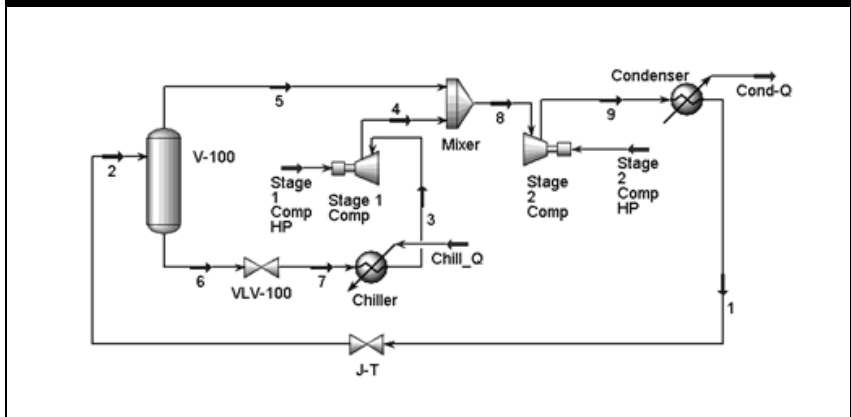
Add the following specifications to the refrigeration loop:

For this Item...	Add this specification...
Stream 1	T = 50°C and Vf = 0.0. 100% Propane
Chiller	Pressure Drop = 7 kPa Q = 1.0e+006 kJ/h
Stream 3	T = -20°C Vf = 1.0
Stream 4	P = 625 kPa
Mixer	Equalize All Pressures
Condenser	Pressure Drop = 35 kPa

Save your case!

3. Refrigerated Gas Plant

Workshop

In this simulation, a simplified version of a refrigerated gas plant will be modeled. The purpose is to find the LTS (Low Temperature Separator) temperature at which the hydrocarbon dew point target is met. The Sales Gas hydrocarbon dew point should not exceed -15°C at 6000 kPa. The incoming gas is cooled in two stages—first by exchange with product Sales Gas in a gas-gas exchanger (Gas-Gas) and then in a propane chiller (Chiller), represented here by a Cooler operation. A Virtual Stream operation will be used to evaluate the hydrocarbon dew point of the product stream at 6000 kPa.

Learning Objectives

Once you have completed this section, you will be able to:

- Install and converge heat exchangers
- Understand logical operations (Virtual Stream and Adjust)
- Use the Case Study tool to perform case studies on your simulation

Prerequisites

Before beginning this section you need to know how to:

- Create a fluid package
- Add streams
- Add unit operations

Process Overview

Chiller

Pressure Drop	35.00	kPa

GasGas

Tube Side Pressure Drop	35.00	kPa
Shell Side Pressure Drop	5.000	kPa
Minimum Approach	5.000	C

ADJ-1

Specified Target Value	-15.00	C

VS-1

Target Vapour Fraction	1.000	
Target Temperature	-15.00	C
Target Pressure	6000	kPa
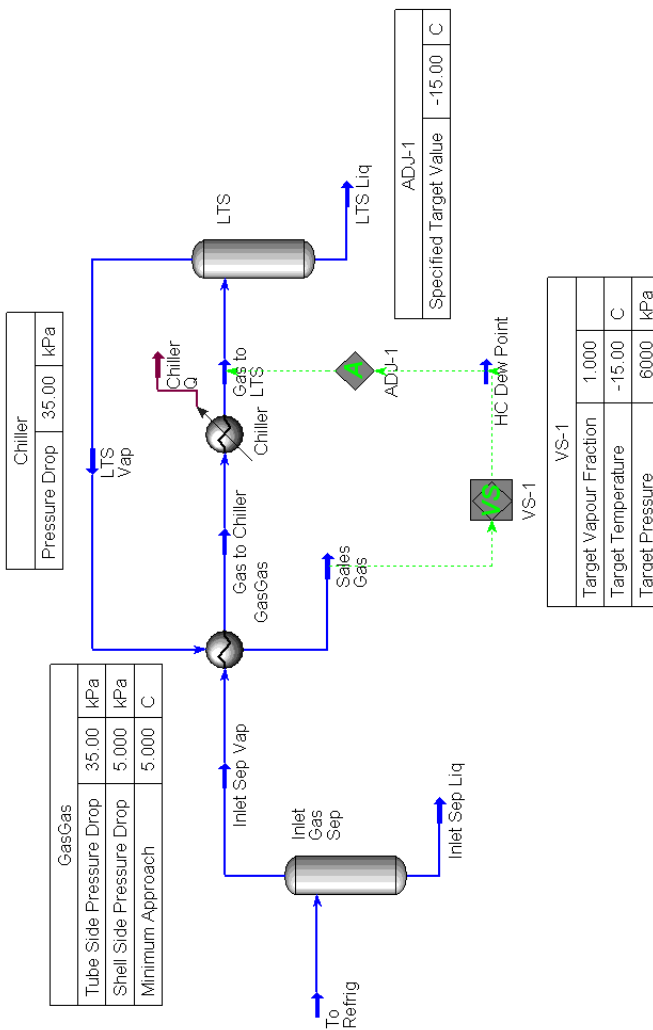
To Refrig

Temperature	15.00	C
Pressure	6200	kPa
Molar Flow	1440	kgmole/h
Comp Mole Frac (Nitrogen)	0.006600	
Comp Mole Frac (H2S)	0.000300	
Comp Mole Frac (CO2)	0.000300	
Comp Mole Frac (Methane)	0.757500	
Comp Mole Frac (Ethane)	0.170900	
Comp Mole Frac (Propane)	0.041300	
Comp Mole Frac (i-Butane)	0.006800	
Comp Mole Frac (n-Butane)	0.010100	
Comp Mole Frac (i-Pentane)	0.002800	
Comp Mole Frac (n-Pentane)	0.002700	
Comp Mole Frac (n-Hexane)	0.000600	
Comp Mole Frac (C7+*)	0.000100	
Comp Mole Frac (H2O)	0.000000	

Building the Simulation

Three tasks are required to build the simulation:

1. Defining component list and fluid package
2. Adding streams and unit operations
3. Adding logical operation (Virtual Stream and Adjust)

Defining the Simulation Basis

For this case, you will be using the Peng-Robinson EOS with the following components:

• Nitrogen	• i-Butane
• H2S	• n-Butane
• CO2	• i-Pentane
• Methane	• n-Pentane
• Ethane	• n-Hexane
• Propane	• C7+*
	• H2O

1. Create a New Case.

2. On the **Fluid Pkgs** tab import the fluid package, **4526.01.GasPlant.fpk**, which you saved in Module 1 (**Getting Started**).

If you want to re-create the fluid package, refer to the first module (**Getting Started**).

Adding a Feed Stream

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

In this cell...	Enter...
Name	To Refrig
Temperature	15°C (60°F)
Pressure	6200 kPa (900 psia)
Flow Rate	1440 kgmole/h (3175 lbmole/hr)
Component	**Mole Fraction**
Nitrogen	0.0066
H2S	0.0003
CO2	0.0003
Methane	0.7575
Ethane	0.1709
Propane	0.0413
i-Butane	0.0068
n-Butane	0.0101
i-Pentane	0.0028
n-Pentane	0.0027
n-Hexane	0.0006
C7+*	0.0001
H2O	0
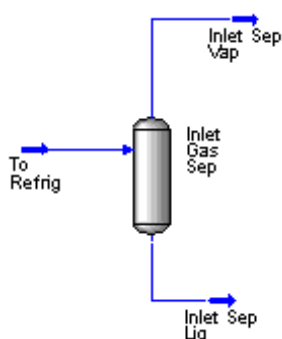
Adding a Separator

There are several ways to add unit operations. For a complete description, see the **Propane Refrigeration Loop** module (**Adding Unit Operations to a Flowsheet** section).

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

On the **Connections** tab, add a **Separator** and enter the following information:

In this cell...	Enter...
Name	Inlet Gas Sep
Feed	To Refrig
Vapour Outlet	Inlet Sep Vap
Liquid Outlet	Inlet Sep Liq

Adding a Heat Exchanger

Heat Exchanger icon

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

1. Double-click the **Heat Exchanger** button on the Object Palette.

2. On the **Connections** page, enter the following information:

The **Tube Side** and **Shell Side** streams can come from different Flowsheets, so for example, you can use Steam Tables for the fluid package on one side of the exchanger and Peng-Robinson on the other side.
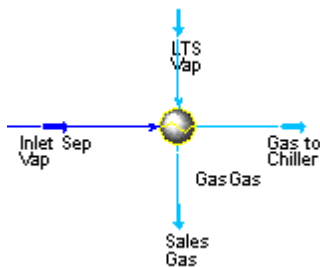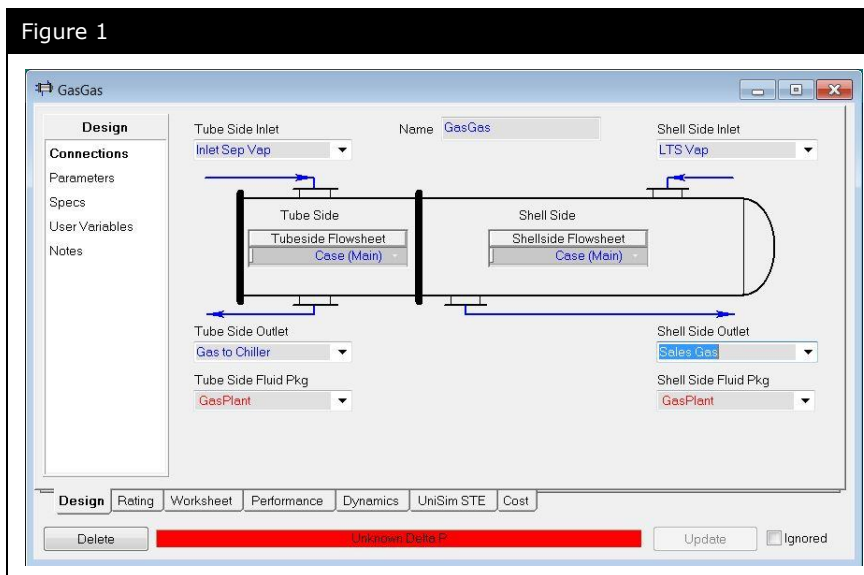
Figure 1

3. Switch to the **Parameters** page. Complete the page as shown in the following figure. Set the **Heat Exchanger Model** to **Exchanger Design (Weighted)**. The pressure drops for the Tube and Shell sides will be **35 kPa (5 psi)** and **5 kPa (1 psi)**, respectively.

Figure 2
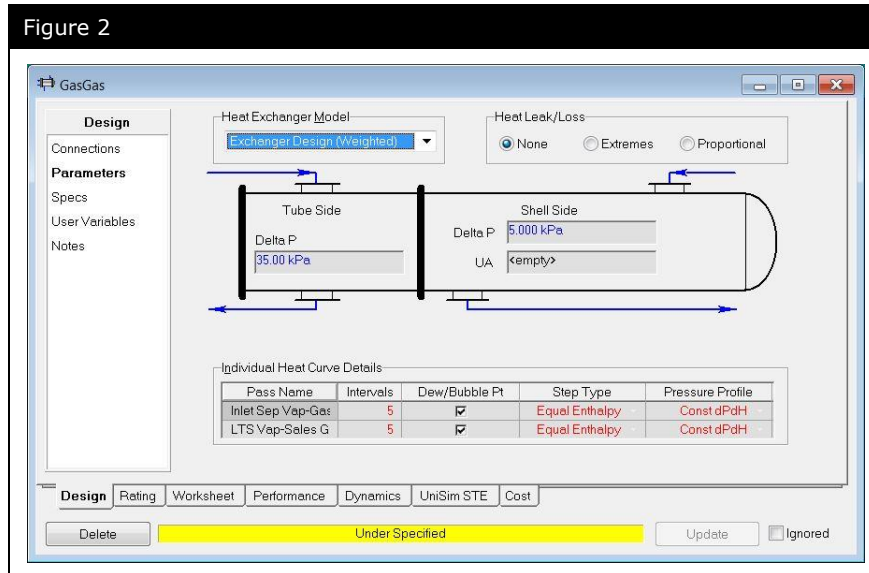
The heat exchanger models are defined as follows:

- **Weighted**. The heating curves are broken into intervals, which then exchange energy individually. An LMTD and UA are calculated for each interval in the heat curve and summed to calculate the overall exchanger UA. The Weighted method is available only for Counter-Current exchangers.

- **End Point**. A single LMTD and UA are calculated from the inlet and outlet conditions. For simple problems where there is no phase change and Cp is relatively constant, this option may be sufficient.

4. Go to the **Specs** page.

To solve the heat exchanger, unknown parameters (flows, temperatures) are manipulated by the solver. Each constraint (specification) will reduce the degrees of freedom by one. The number of constraints (specifications) must equal the number of unknown variables. When this is the case, the degrees of freedom will be equal to zero, and a solution will be calculated.

Two specifications are needed for this exchanger:

- **Heat Balance = 0**. This is a Duty Error specification and is needed to ensure that the heat equation balances. This is a default specification that is always added by UniSim Design so you do not need to supply it.
- **Min Approach = 5°C**. This is the minimum temperature difference between the hot and cold stream.

You can have multiple Estimate specifications. The Heat Exchanger will only use the Active specifications for convergence.

5. To add a specification, click the **Add** button, the **ExchSpec** view appears.

Figure 3
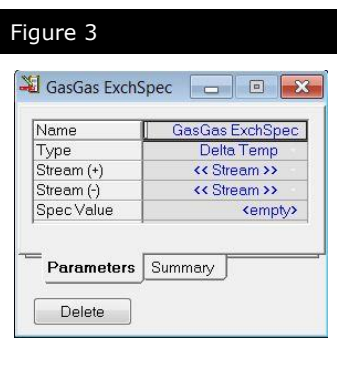
6. Provide the following information:

In this cell...	Enter...
Name	Temp Approach
Type	Min Approach
Pass	Overall
Spec Value	5°C (9°F)

When you change the type of specification, the view will change accordingly. Once all the information has been provided, the view will be as shown below:
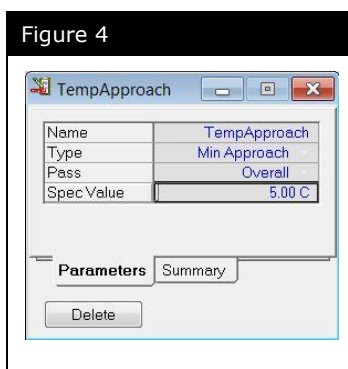
Figure 4

7. Activate the new specification by checking the Active checkbox:

Figure 5
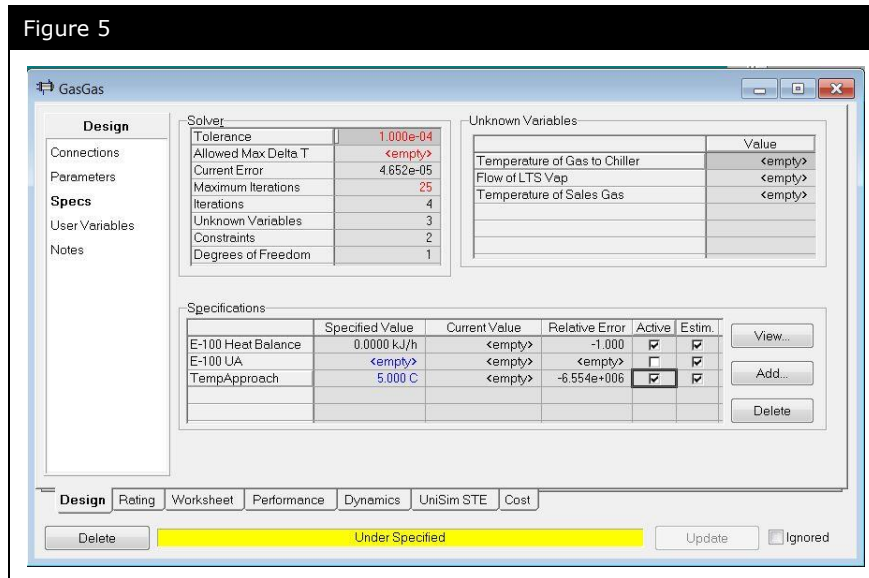
What is the flow rate of Gas to Chiller?

_____

Finishing the Simulation
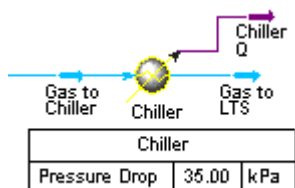
Add the two remaining physical unit operations to complete the simulation.

1. Add a **Cooler** and provide the following information:

In this cell...	Enter...
Connections	
Name	Chiller
Inlet Stream	Gas to Chiller
Outlet Stream	Gas to LTS
Energy Stream	Chiller Q
Parameters	
Delta P	35 kPa (5 psi)
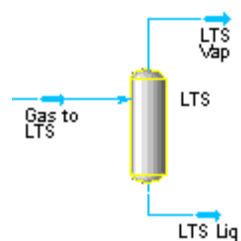
2. Add a **Separator** and provide the following information on the **Connections** tab:

In this cell...	Enter...
Name	LTS
Inlet Stream	Gas to LTS
Vapour Outlet	LTS Vap
Liquid Outlet	LTS Liq

> *What piece of information is required for the LTS separator to solve?*
> _____

In the next section the LTS feed temperature will be varied using an Adjust operation to find a temperature at which the dew point constraint is met. For now, specify the temperature of stream **Gas to LTS** to be **–20°C** (-4°F).

What is the pressure of Sales Gas?
_____

What is the temperature of Sales Gas?
_____

Adding a Virtual Stream

Virtual Stream icon

The Virtual Stream operation provides a general purpose facility to create a live copy of the data from one stream (the Reference stream) to another (the Target stream). The Reference and Target streams must be specified on the **Connections** tab. The Virtual Stream operation may also be used in other cases, for example, to perform flash calculations.

Figure 6

To make a duplicate of a stream, four reference variables must be selected in the **Transfer Information** section of the **Parameters** tab as depicted in Figure 7 below. Composition must be selected, flow (molar or mass) and two of either: vapour fraction, temperature, pressure and enthalpy. Selecting pressure and enthalpy as the last two variables will define the stream uniquely.

Note backward translation from the **Target** Stream to the **Reference** Stream is also possible if the corresponding property of the reference stream is deleted and the property of the target stream is specified instead.

The Virtual Stream is classified with the logical operations on the Object Palette.

The Virtual Stream operation shows green connections because it does not imply a material balance.

Figure 7
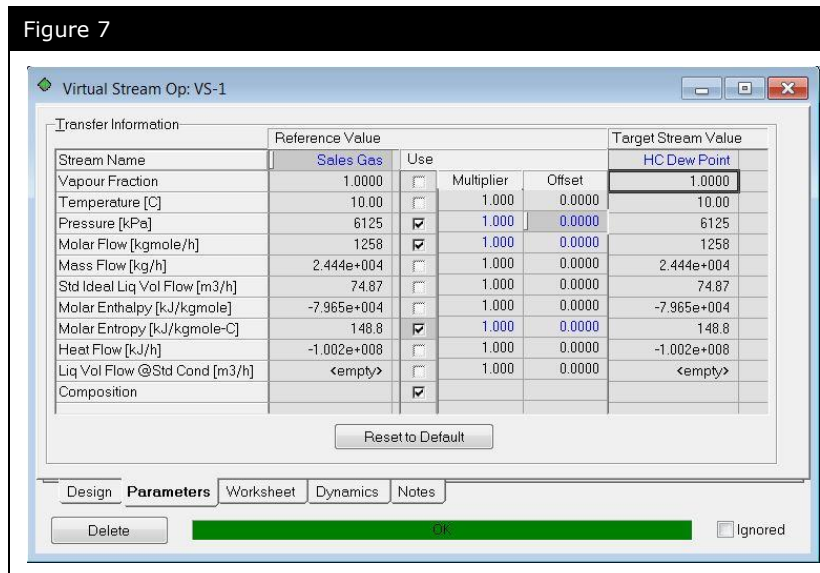
In order to use the Virtual Stream operation to perform flash calculations, composition and flow (molar or mass) must be selected in the **Transfer Information** area of the Virtual Stream Parameters tab. The user will specify the flash variables, vapour fraction, pressure and/or temperature, depending on whether dew or bubble point calculations are the desired target.

1. Double-click on the **Virtual Stream** icon on the Object Palette.
2. Add the following information on the **Connections** tab:

The Virtual Stream operation translates stream data using a multiplier and offset per the following linear formula:

$$Y = M*X + B$$

M=Multiplier, B=Offset

Y is the Target stream data, and X is the Reference stream data.

In this cell...	Enter...
Reference Stream	Sales Gas
Target Stream	HC Dew Point

3. Go to the **Parameters** tab.
4. Select composition and flow (molar or mass).
5. Specify a **Pressure** of **6000 kPa** (**870 psia**) for the stream **HC Dew Point**, and set the **Vapour Fraction** to calculate the **dew point temperature**. This can be done on the **Parameters** tab of the Virtual Stream (Target Value), or on the **Worksheet** tab of the HC Dew Point stream itself. Observe that entering the values in one will populate the other.

Figure 8

What is the dew point temperature?

_____

The required dew point is -15°C, is the current dew point higher or lower?

_____

Assuming pressure is fixed, what other parameter affects the dew point?

_____

How can we change the dew point in the simulation?

_____

Adding the Adjust

Adjust icon

The Adjust operation is a Logical Operation; a mathematical operation rather than a physical operation. It will vary the value of one stream variable (the independent variable) to meet a required value or specification (the dependant variable) in another stream or operation.

1. Double-click on the **Adjust** icon on the Object Palette, the Adjust property view appears.

Figure 9

The Adjusted Variable must always be a user-specified value.

2. Click the **Select Var...** button in the Adjusted Variable group. The Variable Navigator view appears.

3. From the Object list, select **Gas to LTS**. From the Variable list which is now visible, select **Temperature**.

Figure 10

4. Click the **OK** button to accept the variable and return to the Adjust property view.

5. Click the **Select Var...** button in the Target Variable group.

6. Select the object **HC Dew point**, and then select **Temperature** as the target variable.

7. Click the **OK** button to accept the variable and return to the Adjust property view.

8. Enter a value of **-15°C** (5°F) in the Specified Target Value box.

9. The completed **Connections** tab is shown below.

Always work left to right in the **Variable Navigator**. Don't forget you can use the **Object Filter** when the Object list is long.

Figure 11

10. Switch to the **Parameters** tab, and enter **Minimum** and Maximum values of **-20°C** (-4°F) and **0°C** (32°F) respectively:
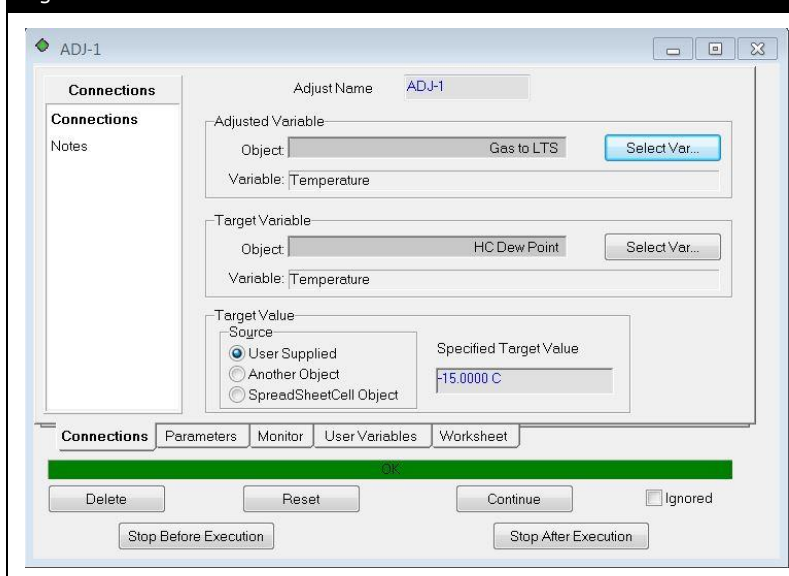
When adjusting certain variables, it is often a good idea to provide a minimum or maximum which corresponds to a physical boundary, such as zero for pressure or flow.

Figure 12
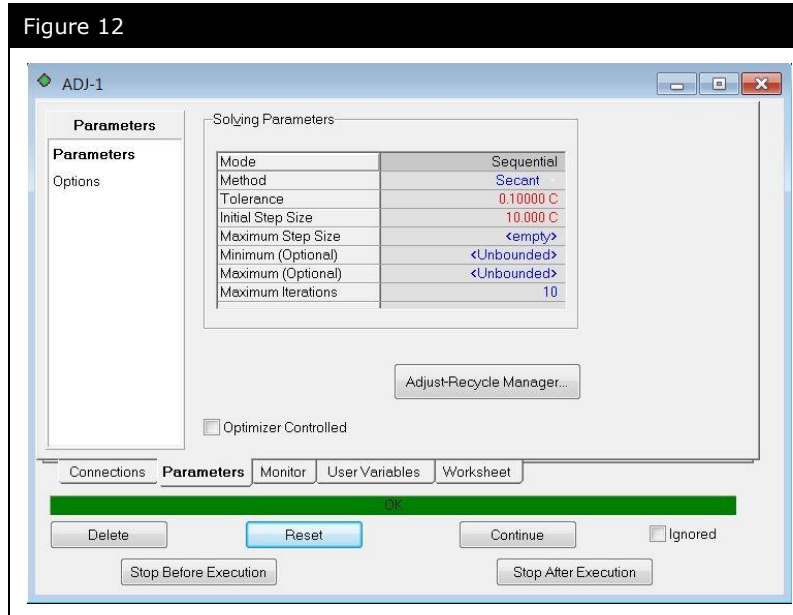
Note the Tolerance and Step Size values. When considering step sizes, use larger rather than smaller sizes. The Secant method works best once the solution has been bracketed and by using a larger step size you are more likely to bracket the solution quickly.

11. To view the progress of the Adjust, go to the **Monitor** tab.

Figure 13
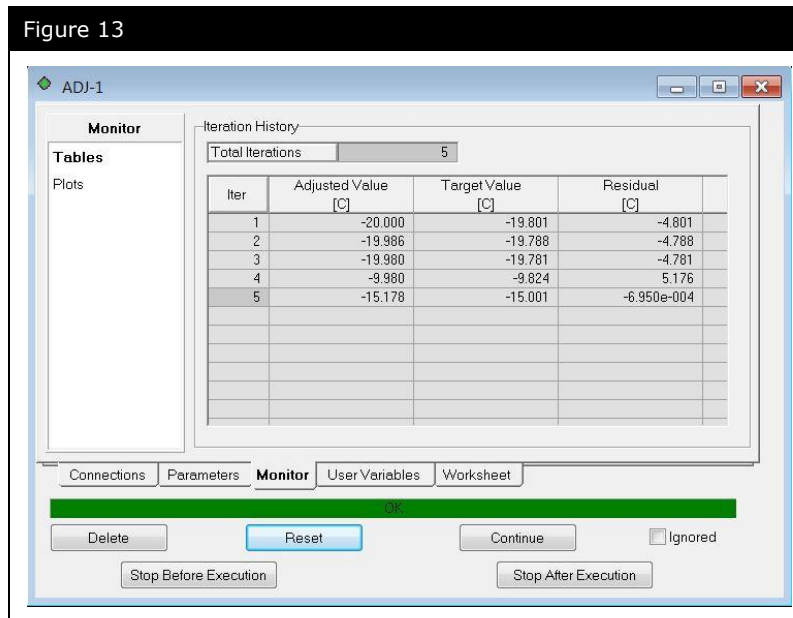
What is the Chiller outlet temperature required to achieve the dew point specification?
_____

Save your case!

Choosing the Adjust Method

In Sequential (i.e. Non-simultaneous) mode the Adjust has a choice of three methods:

- Secant (default)
- Broyden
- Modified Secant

The Modified Secant method was introduced in UniSim Design R380.

In general the Secant is slower but more reliable than the Broyden method. The Modified Secant method includes several enhancements over the original Secant method:

- More efficient control of internal variable bounds and step size.
- Better able to find a bracket for the solution.
- Reverts to Bi-Section search if unable to find a solution otherwise.
- When the calculation is stuck at one variable bound, it will switch to the other bound and continue calculations.

In combination this method allows the Adjust to better cope with the situation where the target variable is invariant over a portion of the adjusted variable range. The Modified Secant method is a good general purpose choice.

Advanced Modeling

Linking the Propane Loop to the Gas Plant

Sub-Flowsheet icon

Once you have completed the Refrigerated Gas Plant example, you can link it to the Propane Loop template.

The Chiller duty, Chiller Q, in the Gas Plant will be linked to the Chiller duty, Chill-Q, in the Propane Refrigeration Loop template.

1. Using the Refrigerated Gas Plant simulation constructed above double-click on the **Sub-Flowsheet** icon on the Object Palette.

2. Click the **Read an Existing Template** button.

3. Navigate to the template file saved in Module 2, **4526.02.C3Loop.utpl**, and click **Open**.

4. In the **Inlet Connections to Sub-Flowsheet** group, connect the External Stream, **Chiller Q** to the Internal Stream **Chill Q**.

If at this point a consistency error occurs consider these questions:

What variable is being transferred from the main flowsheet stream to the sub-flowsheet? Does the sub-flowsheet stream already have a value for this variable? Why?
When the problem is fixed what needs to be done to get UniSim Design to start solving again?

Figure 14
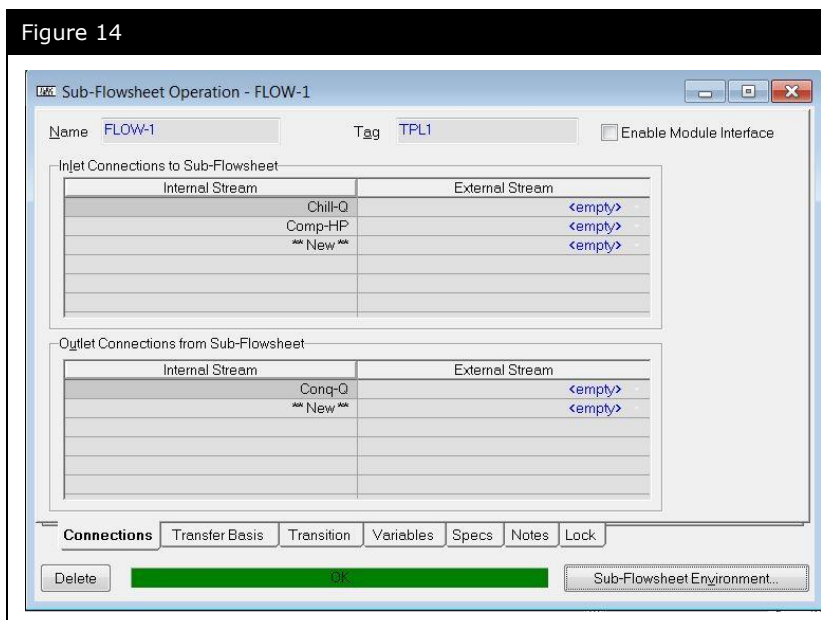
Once the connection is complete, both streams (internal and external) will have the same name (that of the external stream).

What is the flow rate of propane in the Refrigeration Loop?
_____

Exploring the Simulation

Exercise 1: Modifying the Exchanger

The available UA for the Gas-Gas Exchanger is only 2e+005 kJ/°Ch. Make the necessary modifications to your exchanger design to achieve this UA.

How does this affect the LMTD and Temperature Approach?

_____

Challenge

In building the Refrigerated Gas Plant and the Propane Refrigeration Loop you decided to shortcut things and add a single-sided Cooler operation instead of the shell and tube exchanger that will actually be in the plant. This shortcut works for preliminary work, but now you need to replace the cooler with a shell and tube exchanger.

Remember, UniSim Design allows you to attach streams from another flowsheet to either side of the heat exchanger. Using this feature, you should be able to solve this problem with only an exchanger in the Refrigerated Gas Plant (no exchanger in the Propane Refrigeration Loop).

Using the Case Study

Open the starter case: **4526.03.CaseStudyStarter.usc**. This case is the solution to the Challenge problem in Module 2. The Case Study tool allows you to monitor the steady state response of key process variables to changes in your process. You select independent variables to change and dependent variables to monitor. UniSim Design varies the independent variables one at a time, and with each change, the dependent variables are calculated.

The economizer in the propane refrigeration loop results in a saving of energy over the single compression loop. The outlet pressure from the first stage compressor (Stream 4) has a significant effect on the total compression power required. We will use the Case Study to see the effect of changing the first stage compressor outlet pressure on the total power required by the refrigeration loop.

Note: If your case contains any Adjust operations, they must be turned off so that they do not conflict with the Case Study.

Any unit operation can be temporarily removed from the calculations by selecting the **Ignore** checkbox.

1. From the **Tools** menu select **Databook** (or press **CTRL D**), to open the Databook.

Both the independent and the dependent variables are added to the Databook from the Variables tab.

Figure 15
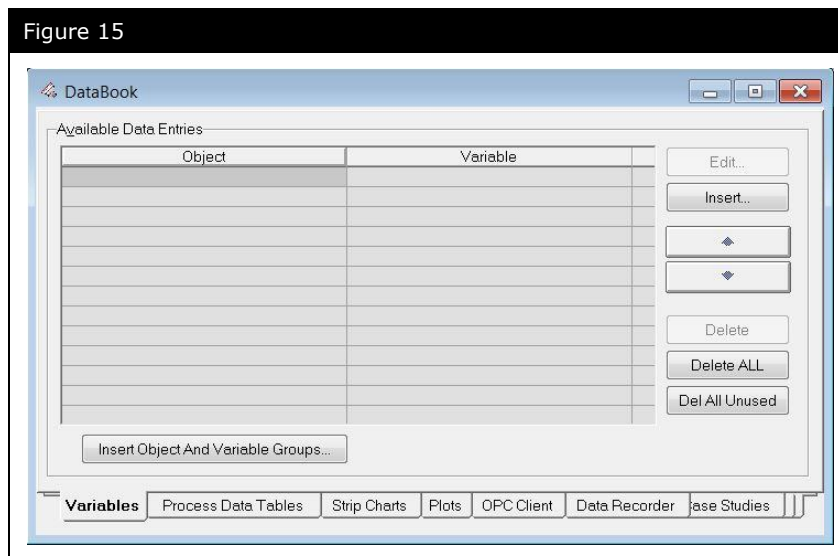
2. On the **Variables** tab, click the **Insert** button to open the Variable Navigator.

3. Select the **Pressure** of stream **4** as the first variable.

4. Click the **Add** button to add the variable.

5. Select spreadsheet **Compressor HP**, cell B4 and click **Add**. Click **Close** to close the Variable Navigator Window.

6. In the Databook, switch to the **Case Studies** tab.

7. Click the **Add** button to add a new Case Study.

8. Select **Stream 4 Pressure** as the Independent Variable and **Compressor HP cell B4** as the Dependent Variable.

Only user-specified variables can be selected as Independent Variables.
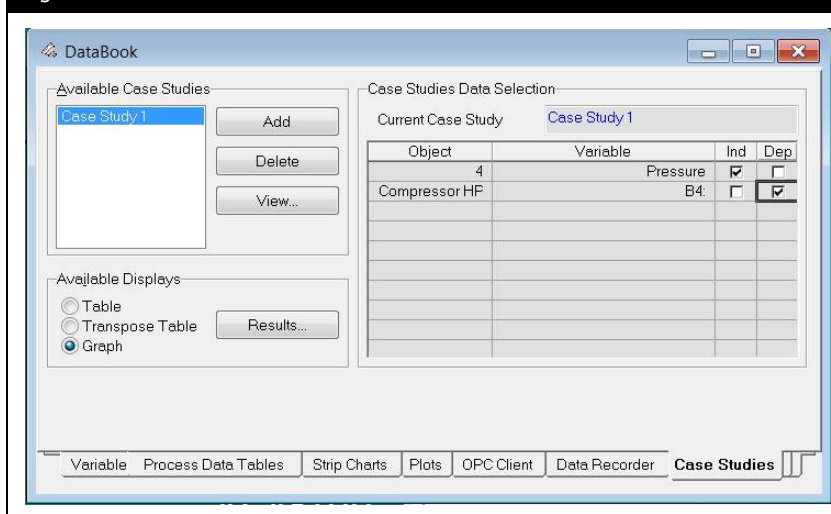
Figure 16

9. Click the **View** button to set up the Case Study.

10. Enter values for **Low Bound, High Bound,** and **Step Size** of 300 kPa (45 psia), 1600 kPa (235 psia) and 50 kPa (5 psi) respectively.

Figure 17
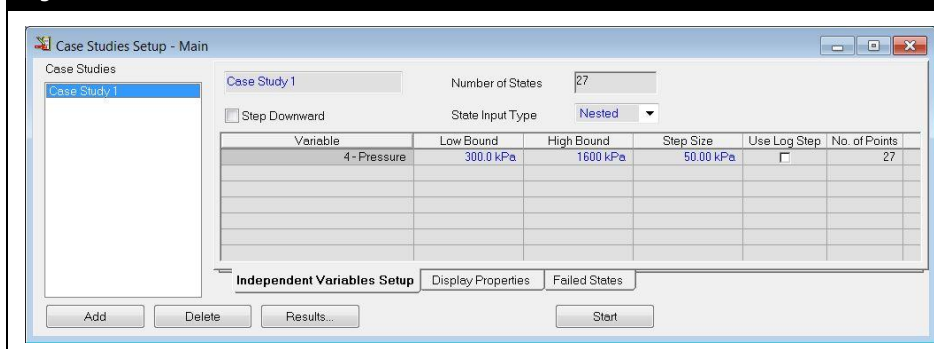
11. Click the **Start** button to begin calculations.

What First Stage compressor outlet pressure (Stream 4) will result in the minimum power usage in the Refrigeration Loop?

_____

4. NGL Fractionation Train

Workshop

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

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

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

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

Learning Objectives

Once you have completed this section, you will be able to:

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

Prerequisites

Before beginning this module, you need to know how to:

- Create a fluid package
- Add streams
- Add unit operations
- Navigate the Workbook interface

Process Overview

Feed1		
Temperature	-95.00	C
Pressure	2275	kPa
Molar Flow	1620	kgmole/h
Comp Mole Frac (Nitrogen)	0.002500	
Comp Mole Frac (CO2)	0.004800	
Comp Mole Frac (Methane)	0.704100	
Comp Mole Frac (Ethane)	0.192100	
Comp Mole Frac (Propane)	0.070600	
Comp Mole Frac (i-Butane)	0.011200	
Comp Mole Frac (n-Butane)	0.008500	
Comp Mole Frac (i-Pentane)	0.003600	
Comp Mole Frac (n-Pentane)	0.002000	
Comp Mole Frac (n-Hexane)	0.000300	
Comp Mole Frac (n-Heptane)	0.000200	
Comp Mole Frac (n-Octane)	0.000100	

Feed2		
Temperature	-85.00	C
Pressure	2290	kPa
Molar Flow	215.0	kgmole/h
Comp Mole Frac (Nitrogen)	0.005700	
Comp Mole Frac (CO2)	0.002900	
Comp Mole Frac (Methane)	0.722700	
Comp Mole Frac (Ethane)	0.117600	
Comp Mole Frac (Propane)	0.075000	
Comp Mole Frac (i-Butane)	0.020400	
Comp Mole Frac (n-Butane)	0.019700	
Comp Mole Frac (i-Pentane)	0.014700	
Comp Mole Frac (n-Pentane)	0.010200	
Comp Mole Frac (n-Hexane)	0.003700	
Comp Mole Frac (n-Heptane)	0.004700	
Comp Mole Frac (n-Octane)	0.002700	

Ex Duty		
Power	583.3	kW

P-100		
Product Pressure	2790	kPa

VLV-100		
Product Pressure	1690	kPa

Column Overviews

DC1: De-Methanizer

Figure 1

Main TS		
Current Number of Stages	10	
Top Stage Pressure	2275	kPa
Bottom Stage Pressure	2310	kPa
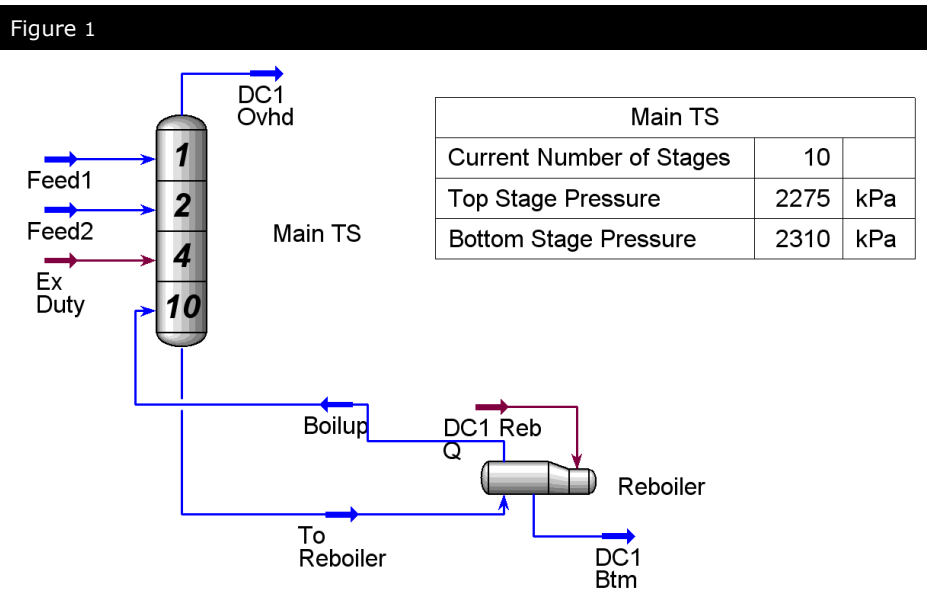
DC2: De-Ethanizer

Figure 2

Main TS		
Current Number of Stages	14	
Top Stage Pressure	2760	kPa
Bottom Stage Pressure	2792	kPa
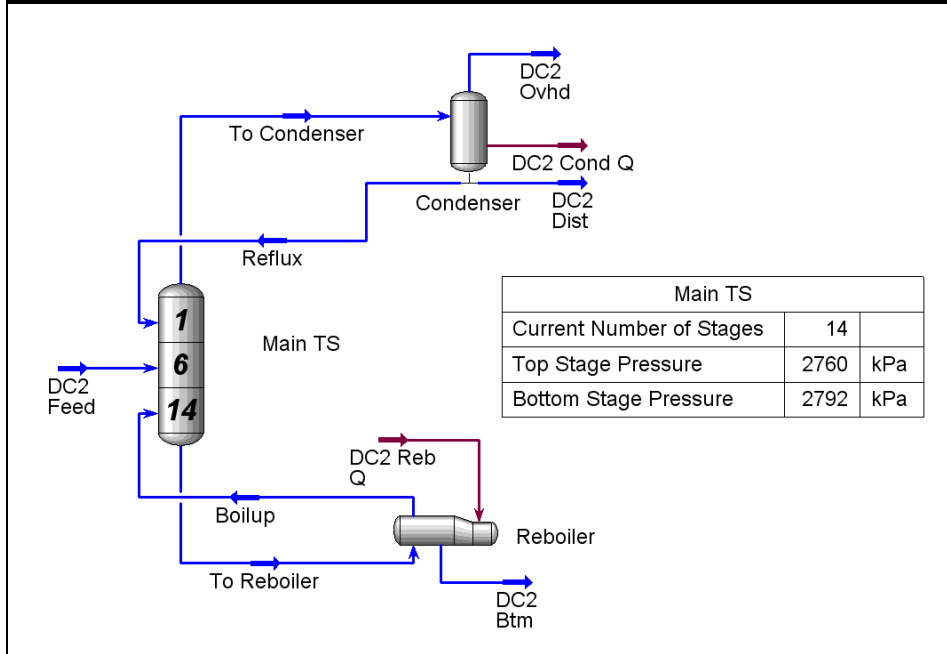
DC3: De-Propanizer

Figure 3

Main TS		
Current Number of Stages	24	
Top Stage Pressure	1620	kPa
Bottom Stage Pressure	1655	kPa
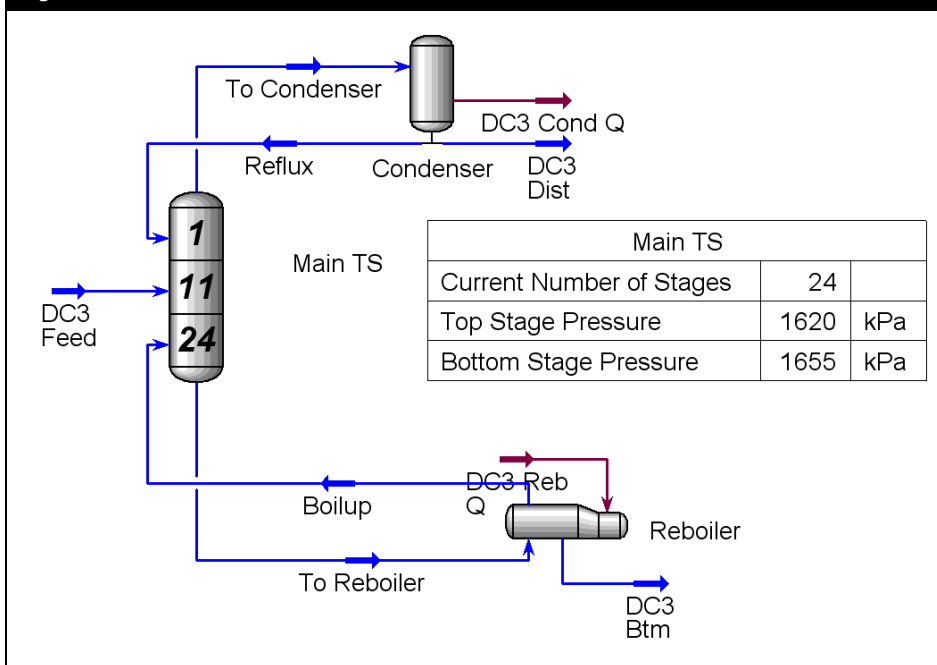
Building the Simulation

Defining the Simulation Basis

1. Start a new case.
2. Select the **Peng-Robinson** EOS.
3. Add the components:

   - Nitrogen
   - CO2
   - Methane
   - Ethane
   - Propane
   - i-Butane

   - n-Butane
   - i-Pentane
   - n-Pentane
   - n-Hexane
   - n-Heptane
   - n-Octane

Enter Simulation Environment icon

4. Enter the **Simulation Environment**.

Adding the Feed Streams

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

In this cell...	Enter...
Name	Feed1
Temperature	-95°C (-140°F)
Pressure	2275 kPa (330 psia)
Flow rate	1620 kgmole/h (3575 lbmole/hr)
Component	**Mole Fraction**
Nitrogen	0.0025
CO2	0.0048
Methane	0.7041
Ethane	0.1921
Propane	0.0706
i-Butane	0.0112
n-Butane	0.0085

In this cell...	Enter...
i-Pentane	0.0036
n-Pentane	0.0020
n-Hexane	0.0003
n-Heptane	0.0002
n-Octane	0.0001

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

In this cell...	Enter...
Name	Feed2
Temperature	-85°C (-120°F)
Pressure	2290 kPa (332 psia)
Flow rate	215 kgmole/h (475 lbmole/hr)
Component	**Mole Fraction**
Nitrogen	0.0057
CO2	0.0029
Methane	0.7227
Ethane	0.1176
Propane	0.0750
i-Butane	0.0204
n-Butane	0.0197
i-Pentane	0.0147
n-Pentane	0.0102
n-Hexane	0.0037
n-Heptane	0.0047
n-Octane	0.0027

Adding the Unit Operations

De-Methanizer

Reboiled Absorber
Column icon

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

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

In this cell...	Enter...
Name	Ex Duty
Energy Flow	2.1e+006 kJ/h (2.0e+06Btu/hr)

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

3. Complete the view as shown below:

The **Input Expert** provides the new user with step by step instruction for defining a column.

Figure 4
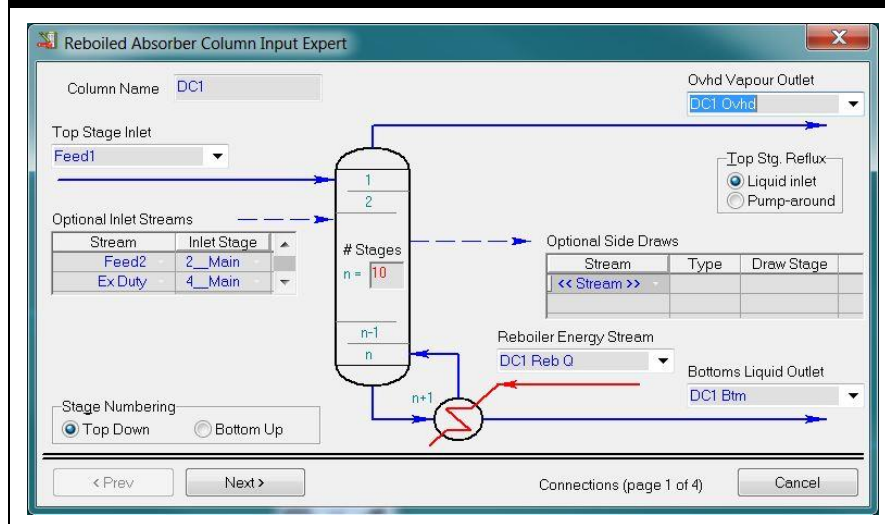
The **Next** button is only available when all of the necessary information has been supplied.

4. Click the **Next** button to proceed to the next page.

5. Supply the following information on the **Pressure Profile** page. If you are using field units, the values will be **330 psia** and **335 psia**, for the Top Stage Pressure and Reboiler Pressure, respectively.

Figure 5
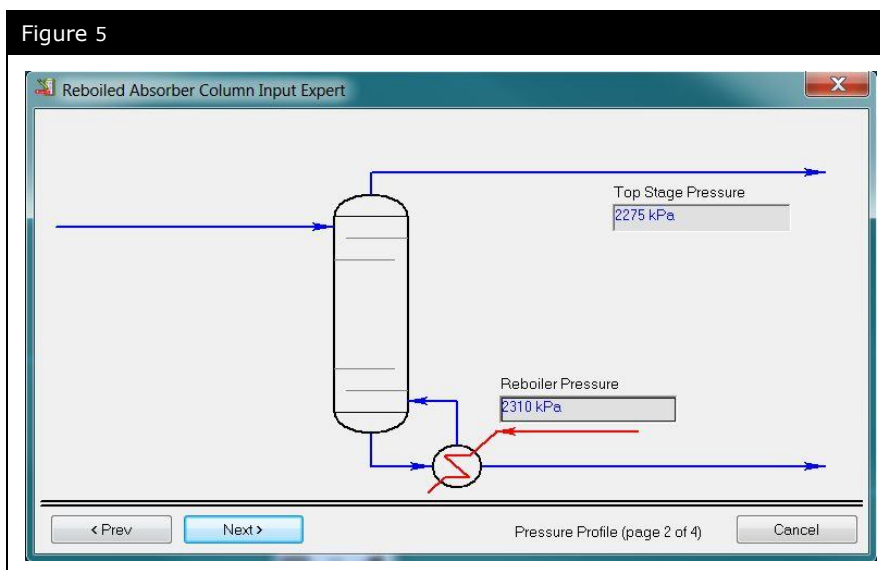
6. Click the **Next** button to proceed to the next page.

7. Enter the temperature estimates shown below. In field units, the top stage temperature estimate will be **-88°C**, and the reboiler temperature estimate will be **27°C**

Temperature estimates are not required for the column to solve but they will aid in convergence.

Figure 6

8. Click the **Next** button to continue.

9. For this case, no information is supplied for the **Boil-up Ratio** on the last page of the Input Expert, so click the **Done** button.
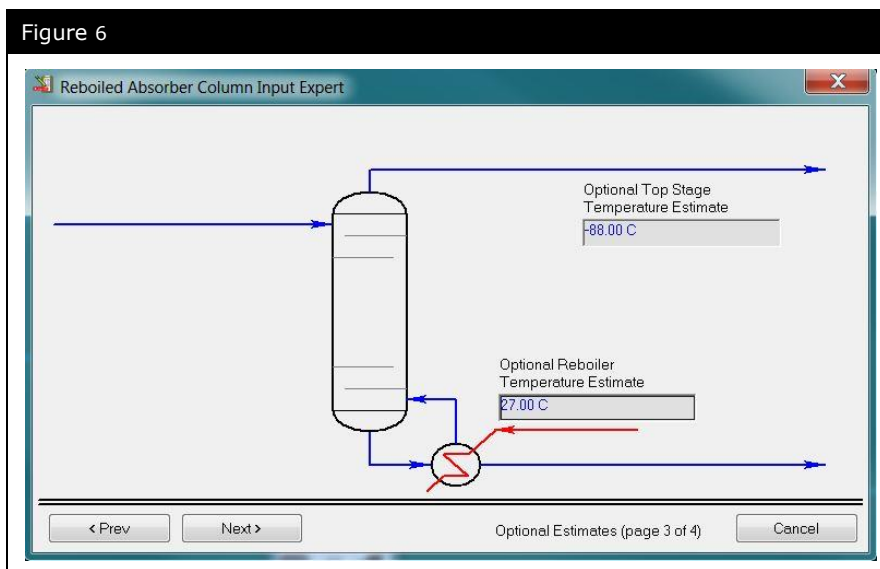
The basic Reboiled Absorber has a single DOF.
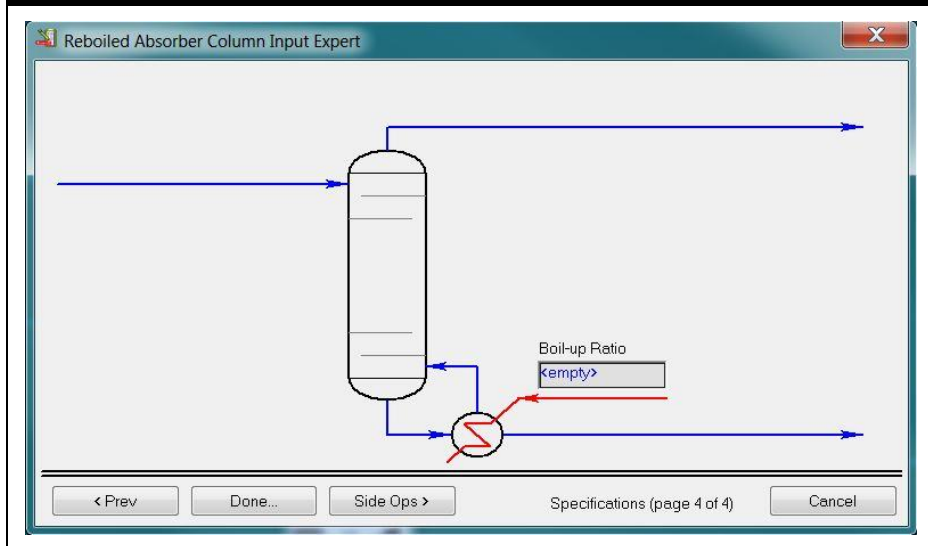
Figure 7

When you click the **Done** button, UniSim Design opens the Column property view. Access the **Monitor** page on the **Design** tab.

Figure 8
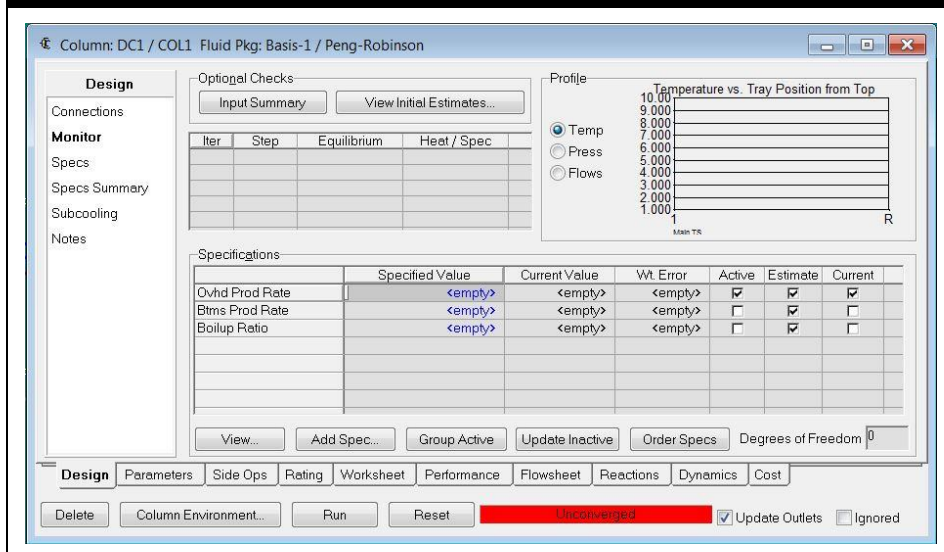
Before you converge the column, make sure that the specifications are as shown above. You will have to enter the value for the **Ovhd Prod Rate** specification. The specified value is **1338 kgmole/h** (2950 lbmole/hr).

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

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

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

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

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

Figure 9
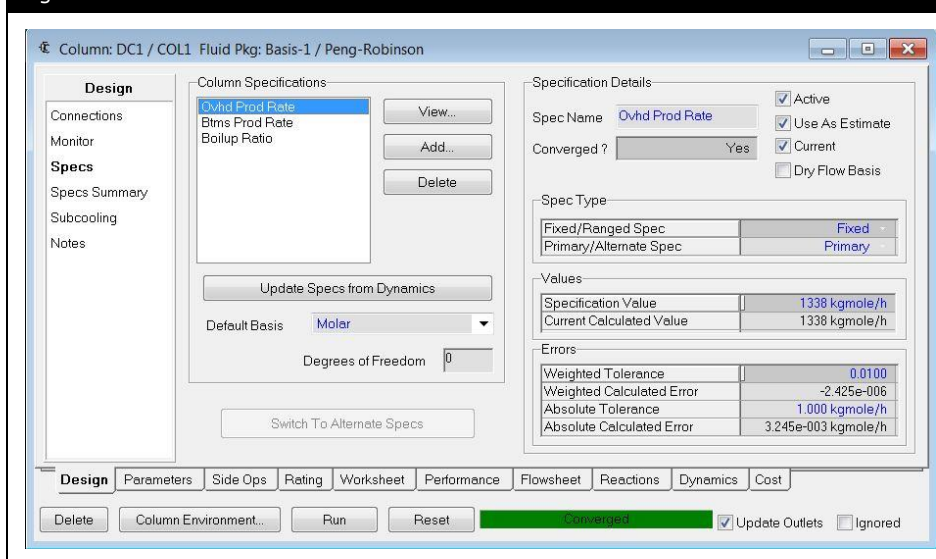
12. Click the **Add** button in the Column Specifications group to create a new specification.

13. Select **Column Component Fraction** from the list that appears.

Figure 10
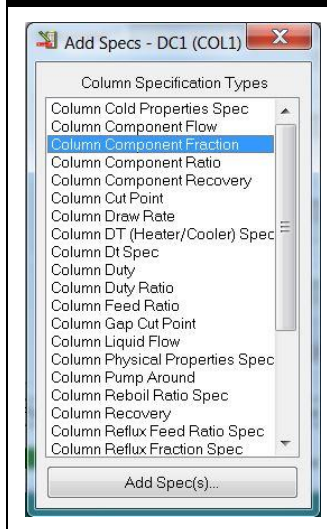
14. Click the **Add Spec(s)...** button.

15. Complete the spec as shown in the following figure.

Figure 11
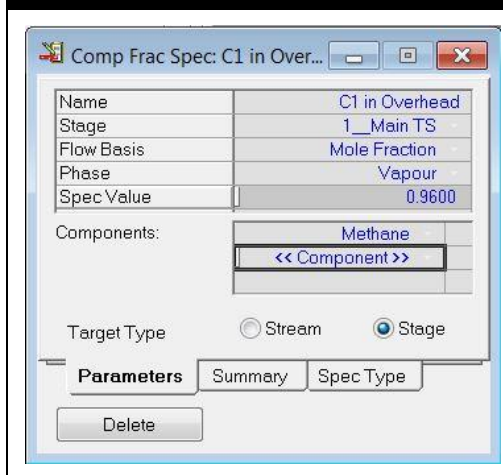
16. When you have finished, close the view.

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

17. Go to the **Monitor** page. De-activate **Ovhd Prod Rate** as an active specification and activate the **Comp Fraction** specification (**C1 in Overhead**) which you created.

What is the flow rate of the overhead product, DC1 Ovhd?

_____

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

Figure 12
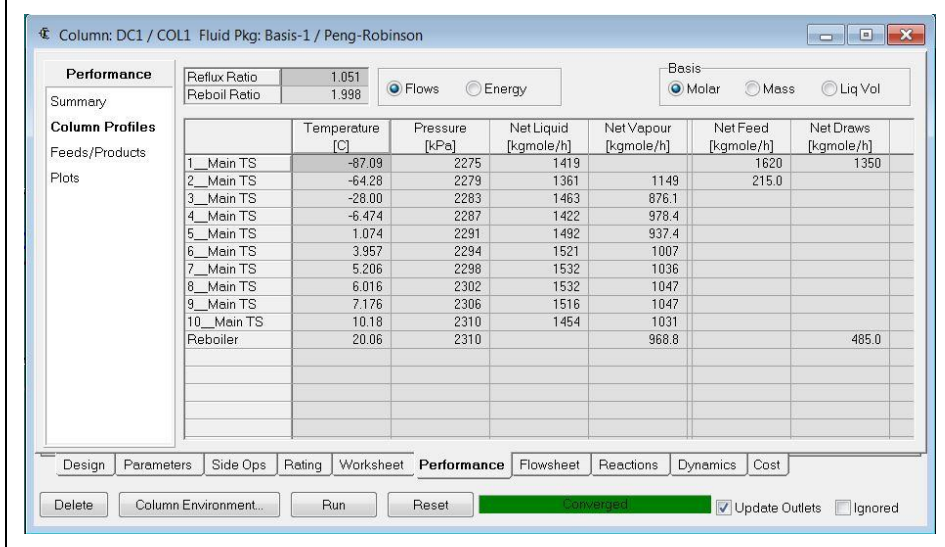
Adding a Pump

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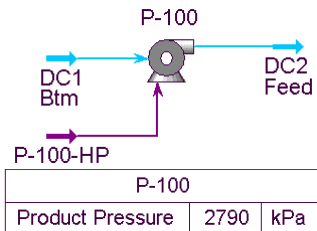
The pump is used to move the De-Methanizer bottom product to the De-Ethanizer.

Install a pump and enter the following information:

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

De-Ethanizer

Distillation Column icon

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

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

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

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

What is the flow rate of Ethane and Propane in DC2 Btm?

Ethane_____, Propane_____

What is the ratio of Ethane/Propane?

_____

3. On the **Specs** page, click the **Add** button to create a new specification.

4. Select **Column Component Ratio** as the **Column Specification Type** and provide the following information:

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

5. On the **Monitor** tab, de-activate the **Ovhd Vap Rate** specification and activate the **C2/C3** specification which you created.

What is the flow rate of DC2 Ovhd?

_____

Adding a Valve

Valve icon

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

Add a Valve operation and provide the following information:
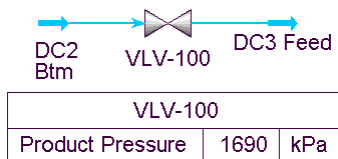
In this cell...	Enter...
Connections	
Inlet	DC2 Btm
Outlet	DC3 Feed
Worksheet	
DC3 Feed Pressure	1690 kPa (245 psia)

De-Propanizer

Distillation Column icon

The De-Propanizer column is represented by a distillation column consisting of 25 separation stages, 24 stages in the tray section plus the reboiler (note: a total condenser does not count as a separation stage). It operates at 1620 kPa (235 psia). There are two process objectives for this column; to produce an overhead product that contains no more than 1.50 mole percent of i-C4 and n-C4, and that the concentration of propane in the bottom product should be less than 2.0 mole percent.

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

In this cell...	Enter...
Connections	
Name	DC3
No. of Stages	24
Inlet Streams/Stage	DC3 Feed/11
Condenser Type	Total
Ovhd Liquid Outlet	DC3 Dist
Bottom Liquid Outlet	DC3 Btm
Reboiler Duty Energy	DC3 Reb Q
Condenser Duty Energy	DC3 Cond Q
Pressures	
Condenser	1585 kPa (230 psia)
Condenser Delta P	35 kPa (5 psi)
Reboiler	1655 kPa (240 psia)
Temperature Estimates	
Condenser	38°C (100°F)
Reboiler	120°C (250°F)
Specifications	
Distillate Rate	110 kgmole/h (240 lbmole/hr)
Reflux Ratio	1.0 (Molar)

2. **Run** the column.

What is the mole fraction of Propane in the product streams?

Overhead_____ Bottoms _____

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

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

4. De-activate the **Distillate Rate** and **Reflux Ratio** specifications.

5. Activate the **i-Butane, n-Butane**, and **Propane** specifications that you created.

Save your case!

Advanced Modeling

The column is a special type of sub-flowsheet in UniSim Design. Sub-flowsheets contain equipment and streams, and exchange information with the parent flowsheet through the connected streams. From the main environment, the column appears as a single, multi-feed, multi-product operation. In many cases, you can treat the column in exactly that manner.

The column sub-flowsheet provides a number of advantages:

- Isolation of the column solver. The Column Environment allows you to make changes and focus on the column without the re-calculation of the entire flowsheet.

- Optional use of different fluid packages. UniSim Design allows you to specify a unique (different from the main environment) fluid package for the column sub-flowsheet. This is useful when a different fluid package is better suited to the column (e.g. a Gas Plant using PR may contain an Amine Contactor that needs to use the Amines Property Package), or the column does not use all of the components used in the main flowsheet and so by decreasing the number of components in the column you may speed up column convergence.

- Construction of custom templates. In addition to the default column configurations which are available as templates, you may define column setups with varying degrees of complexity. Complex custom columns and multiple columns may be simulated within a single sub-flowsheet using various combinations of sub-flowsheet equipment. Custom column examples include, replacement of the standard condenser with a heat exchanger, or the standard kettle reboiler with a thermosyphon reboiler.

- Ability to solve multiple towers simultaneously. The column sub-flowsheet uses a simultaneous solver whereby all operations within the sub-flowsheet are solved simultaneously. The simultaneous solver permits the user to install multiple interconnected columns within the sub-flowsheet without the need for recycle blocks.

The presence of the green "Up Arrow" icon in the toolbar and the Environment Name i.e. (COL1) indicates that you are in the column.

You can enter the column sub-flowsheet by clicking the **Column Environment...** button in the column property view. Once inside the column environment, you can return to the parent environment by either:

Enter Parent Simulation Environment icon

- Clicking the **Enter Parent Simulation Environment** icon in the toolbar.

  or

- Clicking the **Parent Environment...** button in the Column Runner view, as shown below:

Figure 13
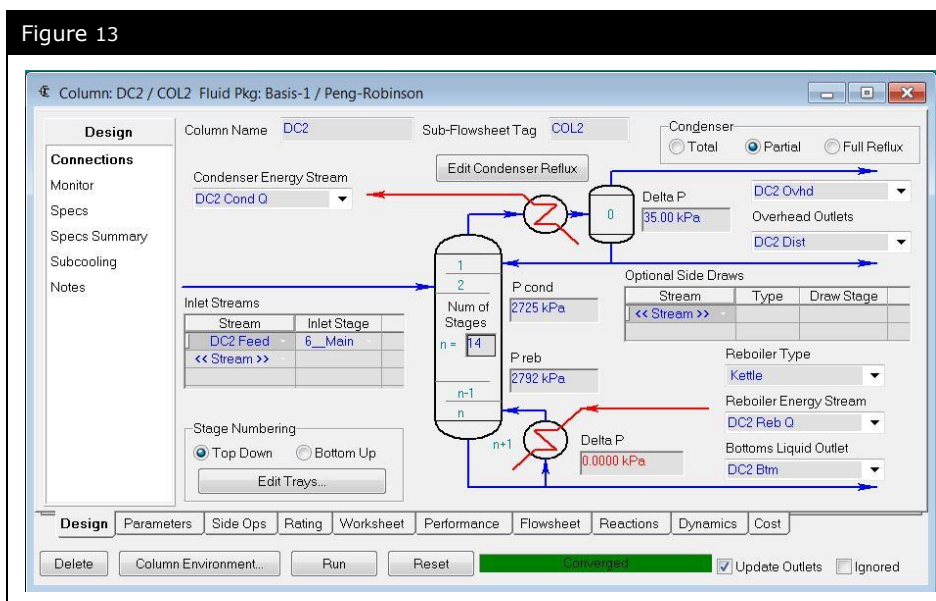
Column Runner icon

If the Column Runner view is not open, click on the **Column Runner** icon in the toolbar.

Exploring the Simulation

Challenge 1

After simulating your De-Methanizer, you have to use UniSim Design to determine the UA for the De-Methanizer Reboiler.

Instead of changing the configuration of the column, you can create an internal stream in the Column Flowsheet (on the **Flowsheet** tab). This stream represents the liquid that flows from the bottom tray to the reboiler, which can then be added to a heat exchanger in the Main Flowsheet. Use steam to exchange heat with the process stream.

Assume that you have 1000 kgmole/h of saturated 100 psi steam available for the shell side and there is a 5 psi pressure drop on the steam side. Your overhead Methane spec of 0.96 (mole) must still be met.

Remember, you will need to add water to your component list.

Challenge 2

For the valve VLV-100 between the De-Ethanizer and the De-Propanizer, the manufacturer provides you with some data about the geometry/size of this valve. Your colleague analyzes this information and comes back with the following data for the valve.

Valve VLV-100	
Valve Manufacturer	ANSI/ISA75.01
Conductance (Cv)	16 USGPM
Characteristic	Linear

The plant operator adds that when the column operates at steady state, valve VLV-100 is opened 30% and the pressure of the inlet stream DC3 Feed should stay within the range of 1600 kPa and 1800 kPa.

Use the information received from your colleague and the P-F Relation specification instead of the Delta P specification for valve VLV-100. Check that the valve stays within the pressure range for stream DC3 Feed when operating at steady state.

5. Oil Characterization

Workshop

The oil characterization function in UniSim Design converts laboratory analyses of condensates, crude oils, petroleum cuts and coal-tar liquids into a series of discrete hypothetical components. These petroleum hypocomponents provide the basis for the property package to predict the remaining thermodynamic and transport properties necessary for fluid modeling.

UniSim Design produces a complete set of physical and critical properties for the petroleum hypocomponents with a minimal amount of information. However, the more information you supply about the fluid, the more accurate these properties will be, and the better UniSim Design will predict the fluid's actual behavior.

In this example, the Oil Characterization option in UniSim Design is used to model a reservoir fluid. The fluid is a combined gas and oil stream.

Learning Objectives

Once you have completed this section, you will be able to:

- Understand oil characterization
- Enter Oil data into UniSim Design and characterize an oil

Prerequisites

Before beginning this module you need to understand the basics of the Fluid Package (refer to the Getting Started module).

Oil Characterization

The Oil Characterization environment provides a location where the characteristics of a petroleum fluid (condensates, crude oils, petroleum cuts, and coal-tar liquids) can be represented by using discrete hypothetical components. Physical, critical, transport, and thermodynamic properties are predicted for each hypocomponent using selected correlations. The fully defined hypocomponent can then be installed in a stream and used in any flowsheet.

The petroleum characterization in UniSim Design accepts different types of information about the oil. The more information you can supply about your sample, the more accurate the representation.

The minimum amount of information that UniSim Design requires to characterize an oil is:

• a laboratory distillation curve

or

• two of the following bulk properties:
  Molecular Weight, Density, or Watson K Factor

Figure 1 illustrates the make-up of a typical oil:

Figure 1
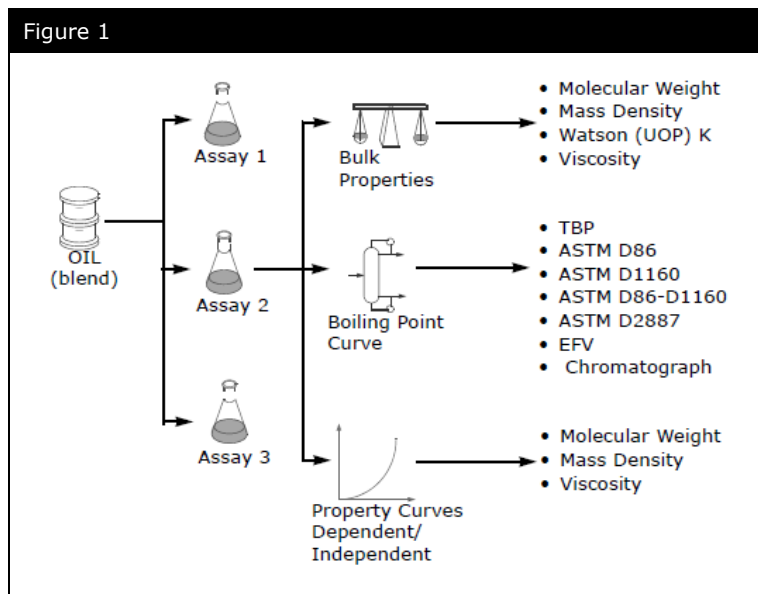
An Oil or Blend is comprised of any number of Assays. Each individual assay contains specific information with respect to the Bulk Properties, Boiling Point Curve and Property Curves.

There are three general steps to follow when creating an oil in UniSim Design:

1. Characterize the assay
2. Generate hypocomponents
3. Install the oil in the flowsheet

Characterize the Assay

UniSim Design defines the hypocomponents by using assay data which you provide. The assay contains all of the petroleum laboratory data, boiling point curves, light ends, property curves and bulk properties. UniSim Design uses the supplied assay data to generate internal TBP, molecular weight and density and viscosity curves (referred to as Working Curves). Just as with fluid packages, assays can be imported and exported to be used in different cases.

The procedure UniSim Design uses to convert assay data into a series of petroleum hypocomponents involves four major internal characterization steps:

- Based on input data, UniSim Design calculates a detailed set of full range Working Curves that include the True Boiling Point (TBP) Temperature, Molecular Weight, Density and Viscosity behavior.
- Next, by using either a default or user-supplied set of cutpoint temperatures, the corresponding fraction for each hypocomponent is determined from the TBP working curve.
- The Normal Boiling Point (NBP), Molecular Weight, Density and Viscosity of each hypocomponent are graphically determined from the working curves.
- For each hypocomponent, UniSim Design calculates the remaining critical and physical properties from designated correlations, based upon the component's NBP, Molecular Weight and Density.

Knowledge of the four phases of the characterization process provides a better understanding of how the input data influences the final outcome of the characterization.

Assay Types

Accurate volatility characteristics are vital when representing a petroleum fluid in your process simulation. For all Distillation Curves, you are required to enter at least 5 data points. UniSim Design accepts the following standard laboratory analytical assay procedures:

For all the distillation curves, you are required to enter at least five data points.

- **True Boiling Point (TBP)**. Performed using a multi-stage batch fractionation apparatus operated at relatively high reflux ratios (15-100 theoretical stages with reflux ratios of 5:1 or greater). TBP distillations conducted at atmospheric or vacuum conditions are accepted by the characterization.

- **ASTM D86**. Distillation employing batch fractionation but conducted using non-refluxed Engler flasks. Generally used for light to medium petroleum fluids. UniSim Design can correct for barometric pressure or cracking effects. You must provide the data on a liquid volume basis.

- **ASTM D1160**. Distillation employing batch fractionation but conducted using non-refluxed Engler flasks. Generally used for heavier petroleum fluids. Curves can be given at atmospheric pressure or corrected for vacuum conditions. You must provide the data on a liquid volume basis.

- **ASTM D86_D1160**. This is a combination of the D86/D1160 distillation data types. You can correct for thermal cracking and enable vacuum distillation for sub-atmospheric conditions. You must provide data on a liquid volume basis.

- **ASTM D2887**. Simulated distillation analysis from chromatographic data. Reported only on a weight percent basis at atmospheric conditions.

- **Equilibrium Flash Vapourization (EFV)**. Involves a series of experiments at constant atmospheric pressure, where the total vapour is in equilibrium with the unvapourized liquid. You must provide data on a liquid volume basis.

During calculations, UniSim Design automatically converts all curves to TBP basis.

- **Chromatographic Analysis**. A gas chromatograph analysis of a small sample of completely vapourized oil, analyzed for paraffin, aromatic, and naphthenic hydrocarbon groups ranging from C6 to C30. Chromatographic analyses may be entered on a mole, mass or liquid volume basis.

The characterization procedure performs its calculations based on an internally calculated TBP curve. If an ASTM or EFV distillation curve is supplied, it is converted to a TBP. If no distillation data is supplied, an average TBP distillation curve is generated, based on the overall MW, density, and Watson (UOP) K factor of the fluid.

Light Ends

Light Ends are defined as pure components with low boiling points. Most notably components in the boiling range of C2 to n-C5. UniSim Design uses your Light Ends data to either define, or replace the low boiling portion of your TBP, ASTM D86, or ASTM D1160 curve with discrete pure components.

UniSim Design provides three options to account for Light Ends:

By pressing the **Light Ends Handling & Bulk Fitting Options** button on the **Input Data** tab of the Assay, UniSim Design allows the user to specify whether the entered distillation curve includes light ends or not.

- **Ignore**. UniSim Design characterizes the Light Ends portion of your sample as hypocomponents. This is the least accurate method and as such, is not recommended.
- **Auto Calculate**. Select this when you do not have a separate Light Ends analysis but you want the low boiling portion of your assay represented by pure components. UniSim Design will only use the pure components you have selected in the fluid package.
- **Input Composition**. Select this when you have a separate Light Ends assay and your petroleum assay was prepared with the Light Ends in the sample. UniSim Design provides a form listing the pure components you selected in the fluid package. This is the most accurate representation method.

Bulk Properties

Bulk Properties for the sample may also be supplied. The bulk properties are optional if a distillation curve or chromatograph have been supplied.

- **Molecular Weight**. This is the Molecular Weight of the bulk sample. It must be greater than 16.
- **Mass Density**. The mass density must be between 250 and 2000 kg/m3. The units for density can be mass density, API or specific gravity, chosen from the drop-down unit list.
- **Watson (UOP) K Factor**. This must be between 8 and 15. The Watson K Factor is an approximate index of paraffinicity, K = ((Mean Avg BP)*(1/3)) / (sp gr 60F/60F).
- **Bulk Viscosities**. Given at two reference temperatures, typically 37.78°C and 98.89°C (100°F and 210°F).

Physical Property Curves

UniSim Design accepts different types of physical property curves:

- Molecular Weight curve

- Density curve
- Viscosity curve

Physical property analyses are normally reported from the laboratory using one of the following two conventions:

- **Dependent Assay Basis**. A common set of assay fractions is used for both the distillation curve and the physical property curve.
- **Independent Assay Basis**. A common set of assay fractions is not used for both the distillation curve and the physical property curve.

If property curve data is not supplied, UniSim Design generates internal curves, calculated/estimated by using correlations designed to model a wide variety of oils.

Property Correlations

UniSim Design allows you to choose from a wide variety of correlations (estimation methods) to determine the properties of the generated hypocomponents. The **Correlation** tab of the Oil Characterization Manager allows you to manage the correlations in your case. From this tab you can easily add new correlation sets and modify existing correlation sets.

The **Default Set** of correlations is as follows:

The **Default Set** of correlations cannot be modified. To specify different correlations or temperature ranges a new correlation set must be created.

Property...	Default Correlation...
MW (Molecular Weight)	Twu
SG (Specific Gravity)	Constant Watson K
Tc (Critical Temperature)	Lee-Kesler
Pc (Critical Pressure)	Lee-Kesler
Acentric Factor	Lee-Kesler
Ideal Enthalpy	Lee-Kesler

In the correlation set window, correlation changes are specified by using the drop-down list in any, or all of the property columns: MW, SG, Tc, Pc, Acc. Factor, and Ideal H.

The Low and High End Temperature cells are the range the selected correlation set is applied to. A property correlation can be changed over an entire range, or a particular correlation can be made valid for a particular boiling point range only by splitting the range. If a range is split, then more than one temperature range will be displayed. As many temperature splits as desired may be added to a correlation set. Temperature splits can be modified any time by simply clicking in the appropriate cell and specifying a new value. Temperature splits may also be removed by merging temperature ranges.

Changes to the assay correlations have no effect when a property curve is supplied (i.e. MW curve). Changes only apply when UniSim Design is estimating the properties.

Changes to the Molecular Weight or Specific Gravity correlations are applied to the assay curve, while the Critical Temperature, Critical Pressure, Acentric Factor and Heat Capacity correlations are applied to the hypocomponent properties of the blend.

Any changes to the correlations for an input assay will result in first the assay being recalculated, followed by any blend that uses that assay. For an existing oil, it will be automatically recalculated/re-cut using the new correlations, and the new components will be installed in the flowsheet.

Hypocomponent Generation/Oil Blending

Cutting and Blending is always a balance of computation speed (less components) against precision (more components).

The Cut/Blend characterization in UniSim Design splits the internal working curves for one or more assays into hypocomponents. The Cut/Blend tab of the Oil Characterization view provides two functions, cutting the oil into hypocomponents and blending two or more Assays into one set of hypocomponents.

Cut Ranges

You have three choices for the Cut Option Selection:

- **Auto Cut** - UniSim Design cuts the assay based on internal values.

Range...	Cuts...
37.78 – 425ºC (100 - 800 ºF)	28 (4 per 37.78ºC or 100ºF)
425 – 650ºC (800 - 1200ºF)	8 (2 per 37.78ºC or 100ºF)
650 – 870ºC (1200 - 1600ºF)	4 (1 per 37.78ºC or 100ºF)

- **User Points** - You specify the number of hypocomponents required. UniSim Design proportions the cuts according to an internal weighting scheme.

Range...	Cuts...
IBP - 425ºC (IBP - 800ºF)	4 per 37.78ºC or 100ºF
425 - 650ºC (800 - 1200ºF)	2 per 37.78ºC or 100ºF
650 - FBP (1200 - FBP)	1 per 37.78ºC or 100ºF

- **User Ranges** - You specify the boiling ranges and the number of cuts per range.

Installing the Oil in the Flowsheet

The final step of the characterization is to transfer the hypocomponent information into the flowsheet.

When different crudes are from very different sources, it is a good idea to blend them separately (create two different blends), and mix them in the Simulation Environment instead of from within the Oil Manager.

The reason is that the Oil Manager in UniSim Design must generate a set of common hypo components that predict the properties of both source oils, which is not necessarily a reasonable expectation for very different crudes.

Building the Simulation

Before you start the characterization process, you must:

- Select a property package
- Add any non-oil components, specifically the light ends that are used in the characterization process

Defining the Simulation Basis

For this module, you will be building on the case that you saved at the end of the Getting Started Module.

Enter Basis
Environment icon

Oil Environment icon

1. Open the case that you saved at the end of the Getting Started Module.

2. Click the **Enter Basis Environment** button to return to the Basis environment.

3. Go to the **Oil Manager** tab and click the **Enter Oil Environment** button. You can also press the **Oil Environment** button on the tool bar. The oil characterization view appears.
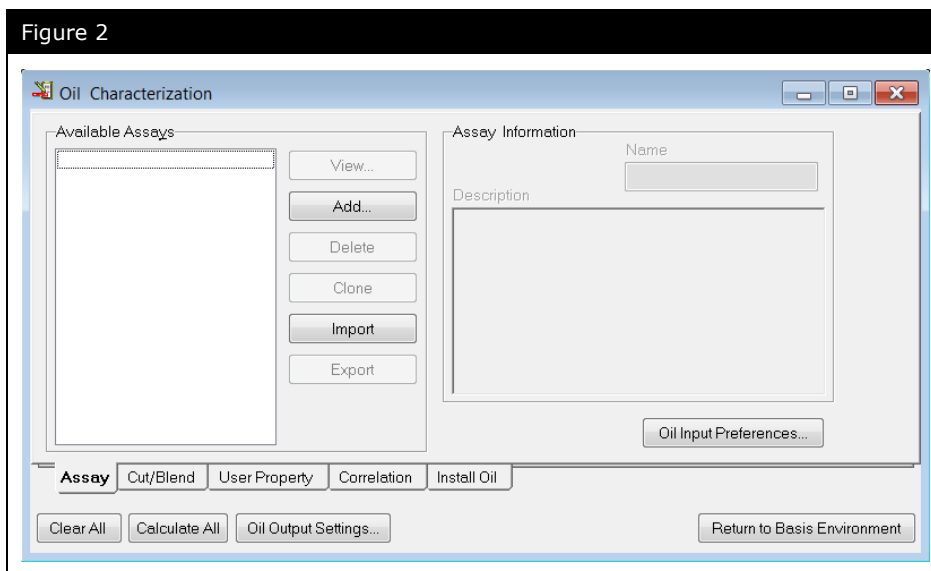
Adding Assay Data

On the Oil Characterizations view:

1. Select the **Assay** tab.
2. Click the **Add** button.
3. The **Input Data** tab of the Assay view appears.
4. In the **Name** cell, change the assay name to **Res-Assay**.
5. In the **Bulk Properties** cell, use the drop-down list to select **Used**.
6. From the **Assay Data Type** drop-down list, select **TBP**.
7. Once the correct type is chosen, additional options should appear. In the Light Ends cell; use the drop-down list to select **Input Composition**. The other cells will not be used in this example.
8. Select the **Light Ends** radio button in the **Input Data** group.
9. Specify the **Light Ends Basis** as **Mole %.** Note that the default basis for Light Ends is **Liquid Volume %;** this must be changed *before* the data is entered.
10. Enter the following data.

For this component...	Enter this Mole %...
Nitrogen	0.48
H2S	0.00
CO2	0.87
Methane	41.83
Ethane	8.87
Propane	7.11
i-Butane	1.47
n-Butane	3.75
i-Pentane	1.25
n-Pentane	1.63
n-Hexane	0.00
H2O	0.00

11. Select the **Distillation** radio button. Change the assay basis from **Mole** to **Liquid Volume**.
12. Click on the **Edit Assay** button to enter the curve as shown below, in either **°C** or **°F**, then click **OK**.

Figure 3
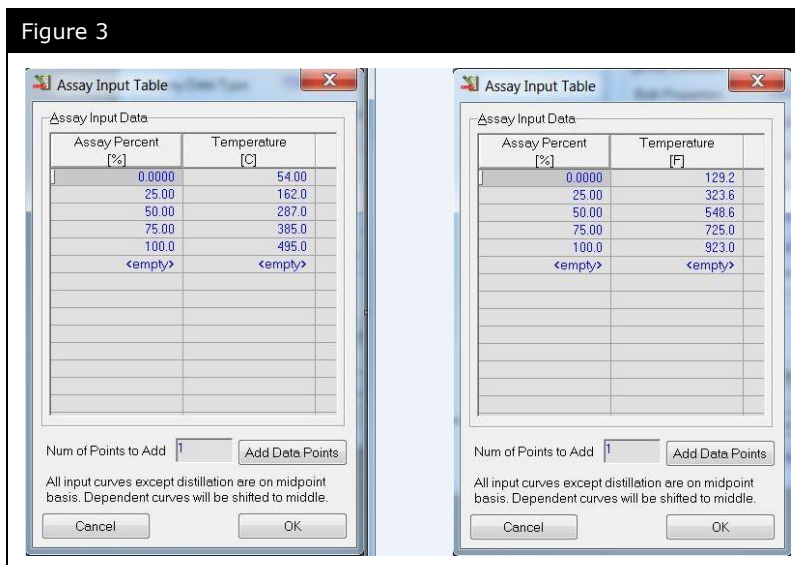
13. Select the **Bulk Props** radio button to enter the following bulk property data:

   - The Molecular Weight is **79.6**
   - The Standard Density is **0.6659 SG_60/60api**

14. Click on the **Light Ends Handling & Bulk Fitting Options** button, and un-check the option for **Curve Incl L.E**. for the distillation curve. This is required because the curve data (assay input data) supplied in Figure 3 does not include the light ends components.

15. Once you have entered all of the data, click the **Calculate** button. The assay status should change to **Assay was Calculated**.

Once the assay is calculated, results are displayed on the **Working Curves** tab. The working curves are regressed from the entered data. The calculation of the blend will be based on these curves.

16. Close the Assay window to return the **Oil Characterization** view. You should still be on the **Assay** tab of the view.

Cutting the Assay

Once the Assay has been calculated, you can cut the Assay into individual hypocomponents.

1. Move to the **Cut/Blend** tab of the Oil Characterization view. Click the **Add** button to create a new Blend.

2. In the Name cell, change the name from the default, Blend-1 to **Res-Fluid**.

3. From the list of Available Assays (there should only be one), select **Res-Assay** and click the **Add-->** button. This adds the Assay to the **Oil Flow Information** table on the **Data** tab, and a blend (cut) will automatically be calculated. The Blend is calculated using the default cut option, **Auto Cut**.

4. Instead of using the default **Auto Cut** option, change the **Cut Option** selection to **User Points** and change the **Number of Cuts** to **5**.

The results can be viewed on the **Tables** tab of the Blend view.

Figure 4

What are the two lowest boiling points for the hypocomponents?

Installing the Oil in the Flowsheet

The final step of the characterization is to transfer the hypocomponent information into the flowsheet.

1. Go to the **Install Oil** tab of the Oil Characterization view. The blend, Res-Fluid appears in the **Oil Install Information** group.

2. In the Stream Name column, enter the name, **GasWell 4**, to which the oil composition will be transferred. UniSim Design will assign the composition of your calculated Oil and Light Ends into this stream, completing the characterization process.

3. Return to the Basis Environment by clicking the **Return to Basis Environment** button.

When you return to the Basis Environment, the hypocomponents that you have generated in the Oil Characterization are placed in the current fluid package. Hypocomponents are named according to the blend group to which they belong and their Normal Boiling Point. For example, a component named NBP[0]94* was generated by the first blend (sequentially numbered within square brackets) in the case and has a boiling point of 94°C.

View the fluid package and examine the individual hypothetical components which make up your oil.

Save your case!

Analyzing the Results

Once you have calculated a blend, you can examine various property and flow summaries for the generated hypocomponents that represent a calculated oil.

In the Oil Environment, open the view for the blend, Res-Fluid.

Tables Tab

The **Tables** tab of the **Blend** contains various information, representing the oil and the components. From the **Table Type** drop-down, you can select different information to display.

- **Component Properties**. When this is selected, choose either **Main Properties** or **Other Properties** from the **Table Control**.
  - **Main Properties**. Provides the normal boiling point, molecular weight, density, and viscosity information for each component in the oil.
  - **Other Properties**. Provides the critical temperature, critical pressure, acentric factor, and Watson K factor for each individual hypocomponent.
- **Component Breakdown**. For the input light ends and each hypocomponent, this provides individual liquid volume %, cumulative liquid volume %, volume, mass, and mole flows.
- **Molar Compositions**. Provides the molar fractions of each light ends component and each hypocomponent in the oil.
- **Oil Properties**. Choose the Basis (Mole, Mass, Liquid Volume) and then the property you want to display.
  - **Distillation**. Provides TBP, D86, D86 Corr, D1160 Vac, and D1160 Atm curves for the oil.
  - **Other Properties**. Provides critical temperature, critical pressure, acentric factor, molecular weight, density, and viscosity ranges for the oil.
  - **User Properties**. Gives all user property curves for the oil.
- **Oil Distributions**. Provides tabular information of how your assay would be distributed in a fractionation column. You can use several kinds of standard fractionation cuts or user defined cuts.

Property Plot Tab

UniSim Design can plot various properties versus liquid volume, mole, or mass percent distilled.

Figure 5
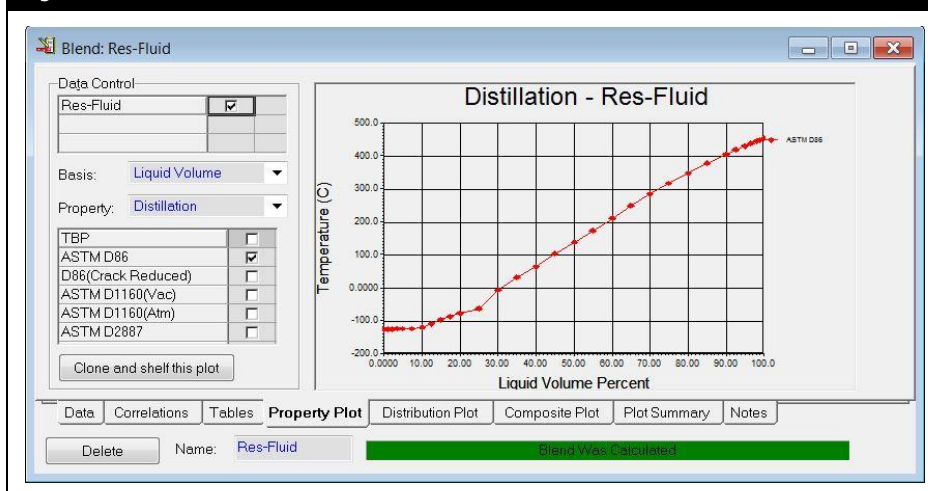
On the **Property Plot** tab, from the **Basis** drop-down list, select Mass, Mole, or Liquid Volume for the X-axis.

From the **Property** drop-down list, choose the property to be plotted on the Y-axis.

- Distillation. You can plot one or more of the following: TBP, D86, D86 (Crack Reduced), D1160 (Vac), D1160 (Atm), or D2887.
- Molecular Weight
- Density
- Viscosity
- Critical Temperature
- Critical Pressure
- Acentric Factor
- User Properties

By clicking on the **Clone and shelf this plot** button, the current plot is copied, renamed and stored. Cloned plots are accessed and viewed from the **Plot Summary tab**.

Distribution Plot Tab

The **Distribution Plot** helps in predicting column products.

The basis for the graphical comparison is made from the Basis drop-down list of three options: Liquid Volume, Mole, and Mass.

The fractionation cut is selected using the radio buttons in the **Cut Input information** group. There are four options:

- **Straight Run**. The Straight Run cut displays the crude column cuts: Off Gas, LSR Naphtha, Naphtha, Kerosene, Light Diesel, Heavy Diesel, Atm Gas Oil and Residue.
- **Cycle Oil**. The Cycle Oil cut displays the Cat Cracker cycle oils: Off Gas, LC Naphtha, HC Naphtha, LCGO, ICGO, HCGO, and Residue Oil.
- **Vacuum Oil**. The Vacuum Oil cut displays the vacuum column cuts: Off Gas, LVGO, HVGO, and five VAC Residue ranges.
- **User Custom**. The User Custom cut allows for the definition of customized temperature ranges. If changes are made to the information in any of the standard fractionation cuts, the radio button will automatically switch to User Custom.

The existing cut temperatures can be edited any time by typing the desired value in the **Cut Input Information table**. If changes are made to the information in any of the fractionation cuts, the radio button will automatically switch to User Custom.

Composite Plot Tab

The **Composite Plot** tab allows you to visually check the match between the input assay data and the calculated property curves. Use Composite Curves to check the accuracy of the input assay data against the hypocomponent properties. The choice for the graphical comparison is made from the **Property** drop-down list.

- TBP or ASTM Distillation Curve
- Molecular Weight Curves
- Mass Density Curves
- Viscosity Curves
- User Property Curve

Viewing the Stream in the Simulation

1. Leave the Oil Environment to return to the Basis Environment.

2. Enter the Simulation Environment

3. If you see a message about HOLDING mode (Figure Figure 6), answer **No**.

Answering Yes to this message will place the solver in Holding mode, meaning no calculations will be performed until the solver is activated via the green traffic light.

Figure 6

UniSim Design

Do you wish to be left in HOLDING mode when entering the Interactive Simulation Environment?

Yes   No   Cancel
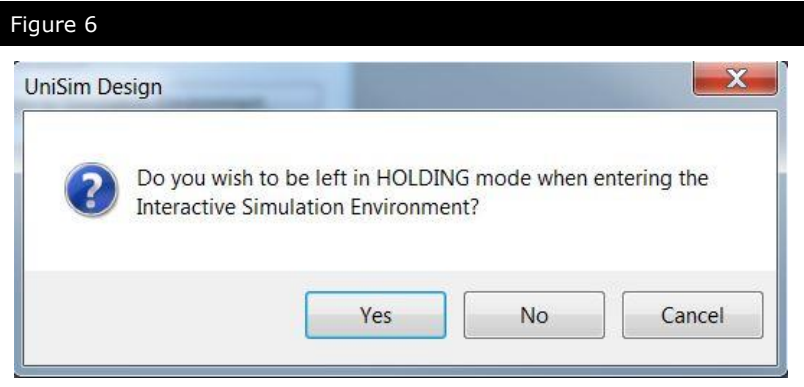
4. Move to the Workbook to view the stream that you created: **GasWell 4**. You can view the stream composition on the Composition page.

If you determine that some of the hypocomponents parameters need to be recalculated, you can return to the Oil Environment at any time to make changes.

Add the following parameters to the stream **GasWell 4**:

- Temperature = **35°C** (95°F)
- Flow rate = **545 kgmole/h** (1200 lbmole/hr)
- Pressure **= 4405 kPa** (639 psia)

Save your case!

Exploring the Simulation

Exercise 1: Composite Plot

You have characterized the assay, specified two bulk properties (Molecular Weight and Density); the hypocomponents have been generated, the assay cut and after installing the oil in the flowsheet (simulation environment), you decide to go back to the oil environment to examine the various Blend plots generated, particularly the Composite Plot.

The Composite Plot can be used to check the accuracy of the calculated hypocomponent properties against the input assay data.

Upon examination of the Composite Plot you observe the calculated hypocomponent data does not match the input assay data you provided at all.

Why doesn't the calculated hypocomponent data match the input curve data supplied in Figure 3? Explain.

_____
_____
_____
_____

Exercise 2: BP Curves Utility

The Boiling Point Curves Utility enables you to obtain the results of a laboratory style analysis for selected simulation streams. This utility is generally used in conjunction with characterized oils from the Oil Manager. The BP Curves Utility calculates simulated distillation data, including TBP, ASTM D86, D86 (Corr), D1160 (Vac), D1160 (Atm), and D2887, as well as critical property data for each cut point and cold property.

The BP Curves Utility is useful for comparing whether there is a good match between the calculated output data and the user supplied input data. The object for the analysis can be a stream, a phase on any stage of a tray section, or one of the phases in a separator, condenser, or reboiler.

From the Simulation Environment, add a BP Curves Utility to stream **GasWell 4**, and compare the results with the input curve data previously provided in Figure 3.

One way to access utilities is by pressing the **CTRL U** hot key to open the **Available Utilities** view.

Are the results from the BP Curves Utility a good match for the input assay data supplied in Figure 3? Why?

_____
_____
_____
_____

Save your case!

Challenge

Recall that the BP Curves Utility is useful for comparing whether there is a good match between the calculated output data and the user supplied input data.

In Exercise 2, it was observed that the calculated hypocomponent property data did not match the input curve data (Figure 3) at all because the input assay data did not include light ends, while the calculated data did.

To allow a true comparison, generate a BP curve for stream **GasWell 4** which does not contain any light ends and compare the results with the input assay data.

Using a Component Splitter to remove the light ends from the stream will facilitate this exercise.

The Component Splitter is an operation that separates a material feed stream into two component streams based on the parameters and component split fractions that you supply.

Note: specifying product stream flash parameters (vapour fraction, temperature and/or pressure), and an energy stream is not required to obtain the resulting BP curve.

What are the calculated temperatures of the fluid without light ends, at the 50% and 75% cut points?

_____

How do the results of the BP Curves utility applied to a stream without Light Ends compare to the input assay data supplied in Figure 3?

_____

6. Two-Stage Compression

Workshop

This example demonstrates a typical application of the recycle operation. Feed gas enters the compressor station at 35°C (95°F) and 1725 kPa (250 psia). The gas is to be delivered at 6900 kPa, and it is to be compressed in two stages. Each stage consists of a knockout drum, a compressor, and a cooler. Liquids from each separator are recycled back to the previous stage, after the pressure has been reduced. A pipe segment is added to the process product stream, and overall material and energy balance checks are performed using UniSim Design's Simulation Balance Tool.

Learning Objectives

Once you have completed this section, you will be able to:

- Use the recycle operation in UniSim Design
- Choose suitable tear locations for recycles
- Add and specify a pipe segment
- Use the Simulation Balance Tool

Prerequisites

Before beginning this module you need to know how to add streams and operations.

Process Overview

To Compression

Temperature	35.00	C
Pressure	1725	kPa
Molar Flow	5000	kgmole/h
Comp Mole Frac (Nitrogen)	0.007500	
Comp Mole Frac (CO2)	0.014700	
Comp Mole Frac (Methane)	0.506900	
Comp Mole Frac (Ethane)	0.145100	
Comp Mole Frac (Propane)	0.072500	
Comp Mole Frac (i-Butane)	0.065200	
Comp Mole Frac (n-Butane)	0.057800	
Comp Mole Frac (i-Pentane)	0.051500	
Comp Mole Frac (n-Pentane)	0.043100	
Comp Mole Frac (n-Hexane)	0.035700	

Mixer 1

Equalize Pressures	Yes

Mixer 2

Equalize Pressures	Yes

Stage 1 Cooler

Product Temperature	50.00	C
Pressure Drop	0.0000	kPa

Stage 2 Cooler

Product Temperature	50.00	C
Pressure Drop	0.0000	kPa

Stage 1

Product Pressure	3450	kPa
Adiabatic Efficiency	75	

Stage 2

Product Pressure	6900	kPa
Adiabatic Efficiency	75	

LetDown 1

Product Pressure	1725	kPa

LetDown 2

Product Pressure	3450	kPa

Building the Simulation

Defining the Simulation Basis

1. Start a new case, set up a fluid package using the Peng-Robinson EOS with the following components:

- Nitrogen
- CO2
- Methane
- Ethane
- Propane

- i-Butane
- n-Butane
- i-Pentane
- n-Pentane
- n-Hexane

Starting the Simulation

2. Add a new Material stream with the following values:

In this cell...	Enter...
Name	To Compression
Temperature	35°C (95°F)
Pressure	1725 kPa (250 psia)
Molar Flow	5000 kgmole/h (11000 lbmole/hr)
Component	**Mole Fraction**
Nitrogen	0.0075
CO2	0.0147
Methane	0.5069
Ethane	0.1451
Propane	0.0725
i-Butane	0.0652
n-Butane	0.0578
i-Pentane	0.0515
n-Pentane	0.0431
n-Hexane	0.0357

Build the Simulation without the Recycle Operations

3. Install a Mixer with the following values:
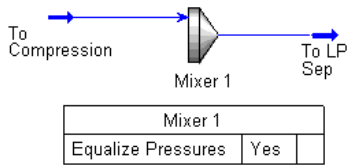
In this cell...	Enter...
Connections	
Name	Mixer 1
Inlet	To Compression
Outlet	To LP Sep
Parameters	
Pressure Assignment	Equalize All

4. Add a Separator with the information shown below:
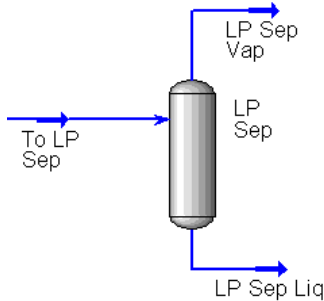
In this cell...	Enter...
Connections	
Name	LP Sep
Inlets	To LP Sep
Vapour Outlet	LP Sep Vap
Liquid Outlet	LP Sep Liq

5. Add a Compressor with the following values:
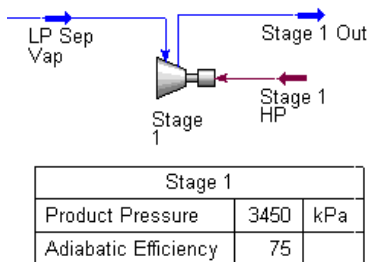
In this cell...	Enter...
Connections	
Name	Stage 1
Inlet	LP Sep Vap
Outlet	Stage 1 Out
Energy	Stage 1 HP
Parameters	
Adiabatic Efficiency	75% (default)
Worksheet	
Stage 1 Out, Pressure	3450 kPa (500 psia)

6. Install a Cooler with the values listed in the following table:
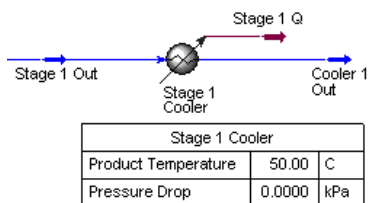
In this cell...	Enter...
Connections	
Name	Stage 1 Cooler
Inlet	Stage 1 Out
Outlet	Cooler 1 Out
Energy	Stage 1 Q
Parameters	
Pressure Drop	0 kPa
Worksheet	
Cooler 1 Out, Temperature	50°C (125°F)

Stage 1 Cooler		
Product Temperature	50.00	C
Pressure Drop	0.0000	kPa

7. Add a Mixer operation to your case.
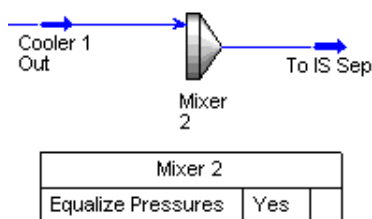
In this cell...	Enter...
Connections	
Name	Mixer 2
Inlet	Cooler 1 Out
Outlet	To IS Sep
Parameters	
Pressure Assignment	Equalize All

Mixer 2		
Equalize Pressures	Yes	

8. Install a Separator with the following information:
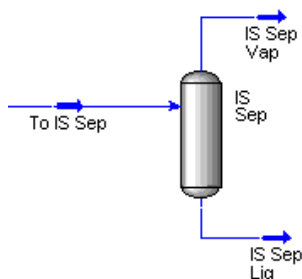
In this cell...	Enter...
Connections	
Name	IS Sep
Inlet	To IS Sep
Vapour Outlet	IS Sep Vap
Liquid Outlet	IS Sep Liq

9. Add a Valve with the following information.
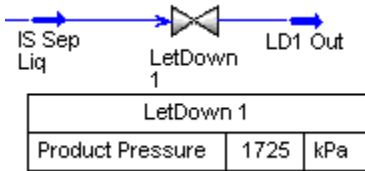
In this cell...	Enter...
Connections	
Name	LetDown 1
Inlet	IS Sep Liq
Outlet	LD1 Out
Worksheet	
LD1 Out, Pressure	1725 kPa (250 psia)

10. Install a Compressor with the values shown below:
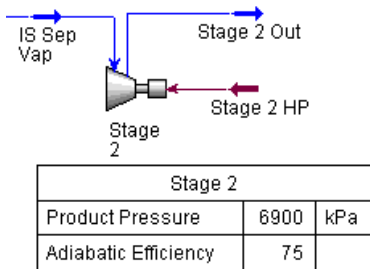
In this cell...	Enter...
Connections	
Name	Stage 2
Inlet	IS Sep Vap
Outlet	Stage 2 Out
Energy	Stage 2 HP
Parameters	
Adiabatic Efficiency	75% (default)
Worksheet	
Stage 2 Out, Pressure	6900 kPa (1000 psia)

11. Install a Cooler operation to the case.
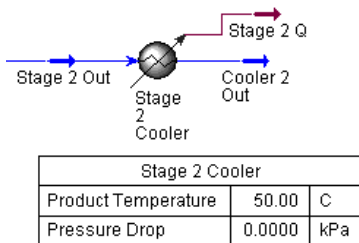
In this cell...	Enter...
Connections	
Name	Stage 2 Cooler
Inlet	Stage 2 Out
Outlet	Cooler 2 Out
Energy	Stage 2 Q
Parameters	
Pressure Drop	0 kPa
Worksheet	
Cooler 2 Out, Temperature	50°C (125°F)

12. Add a Separator with the following values:
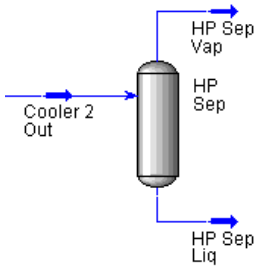
In this cell...	Enter...
Connections	
Name	HP Sep
Inlet	Cooler 2 Out
Vapour Outlet	HP Sep Vap
Liquid Outlet	HP Sep Liq

13. Install a Valve with the following information:
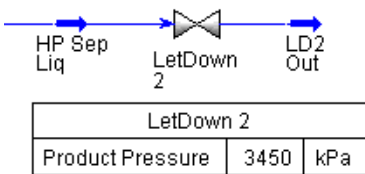
In this cell...	Enter...
Connections	
Name	LetDown 2
Inlet	HP Sep Liq
Outlet	LD2 Out
Worksheet	
LD2 Out, Pressure	3450 kPa (500 psia)

The only operations missing at this point are the Recycles.

14. **Save** your case as 4526.06.TwoStageCompression.usc

Save your case!

Installing the Recycles

Recycle Icon

The UniSim Design Recycle logical operation is used to solve looped systems where downstream material is mixed back in upstream in the process.

UniSim Design employs a non-sequential solving method, which allows information to be propagated both upstream and downstream. This allows some looped systems to be solved explicitly (particularly heat recycles, and refrigeration loops). However for material recycles when downstream material is mixed back in upstream, a Recycle operation is needed.

Recycles are sometimes also known as 'Tears'.

The Recycle operation allows UniSim Design to solve looped system iteratively. A set of conditions are assumed and used to solve the recycle loop. The assumed values are compared with the calculated values and updated. This is repeated until the values match within a specified tolerance. The Recycle operation allows information to be transferred both forwards and backwards (i.e. the assumed value to be in either the outlet or inlet stream), although usually information is only transferred forwards (i.e. assumed value in outlet). In this workshop the recycles will use this mode of operation.

When the Recycle operation is first added, initial estimates need to be provided for all the assumed values. Typically this is done by allowing UniSim Design to solve before closing the recycle loop. This is illustrated in the Workshop.

The following steps take place during the convergence process:

- UniSim Design uses the conditions of the *assumed* stream (usually outlet) and solves the flowsheet up to the *calculated* stream (usually inlet).

- UniSim Design then compares the values of the *calculated* stream to those in the *assumed* stream.

- Based on the difference between the values, UniSim Design modifies the values in the calculated stream and passes the modified values to the *assumed* stream.

- The calculation process repeats until the values in the *calculated* stream match those in the *assumed* stream within specified tolerances.

Examine streams LD1 Out and LD2 Out. Can the values in these streams be used as the guess for the Recycle outlet?

_____

	LD1 Out	LD2 Out
Temperature		
Pressure		
Flow		
Is Composition Known?		

Notice that both LetDown Valve outlets (also the Recycle Inlets) are known. This will be a good starting point for the Assumed stream (the guess of the Recycle).

15. Add the first Recycle by double-clicking on the **Recycle** icon in the Object Palette.

Recycle icon

Connections Page

16. Supply the Name, Feed and Product information as shown:

Figure 1
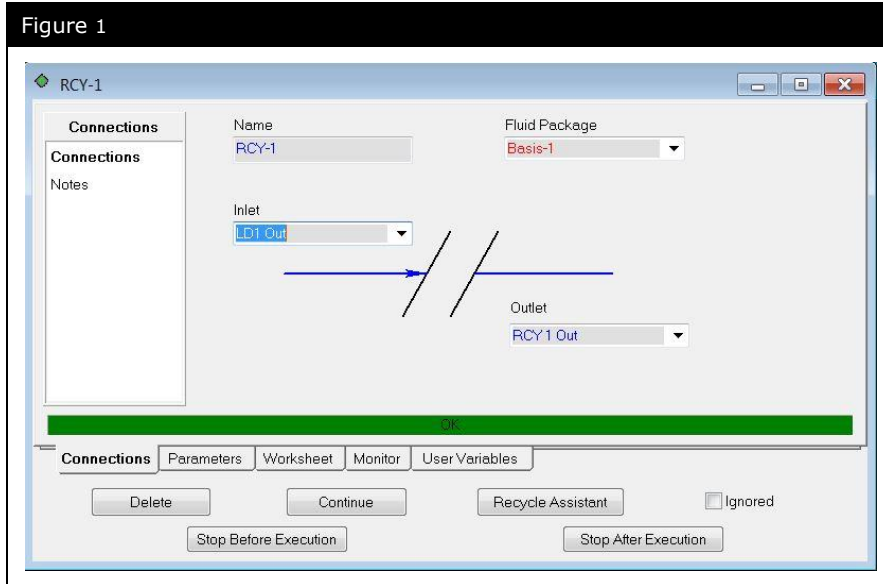
Parameters Tab

Figure 2
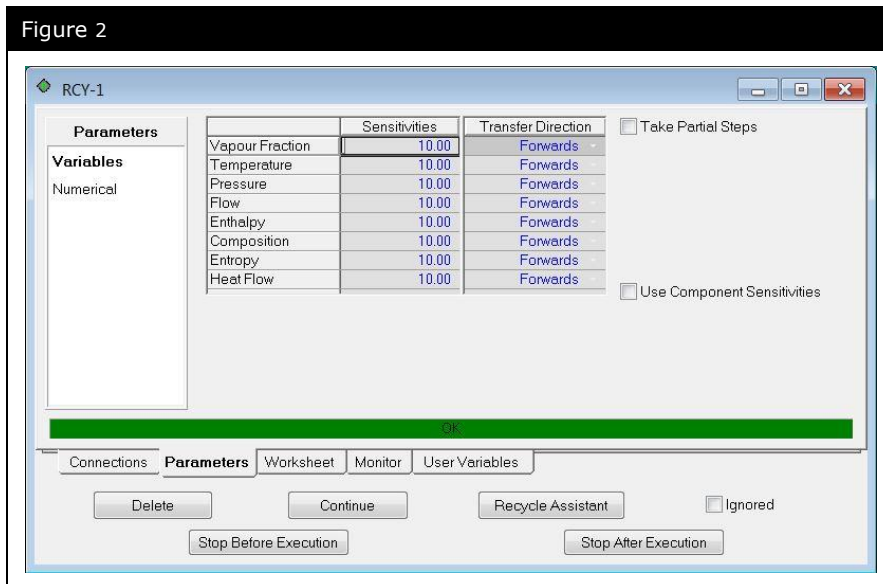
The smaller the tolerance value, the tighter the tolerance. Generally it is a good idea to start with the default tolerance until you have a converged solution and then tighten the tolerance.

UniSim Design allows you to set the convergence criteria or tolerance for each of the Recycle variables. In addition, the direction of transfer of information can be set to **Forwards** or **Backwards**, or **Not Transferred**. In general you will want to leave the transfer as **Forwards**. In this example, leave everything at the default.

Numerical Page

This page contains the numerical options for the Recycle, which control how it is solved numerically.

Figure 3
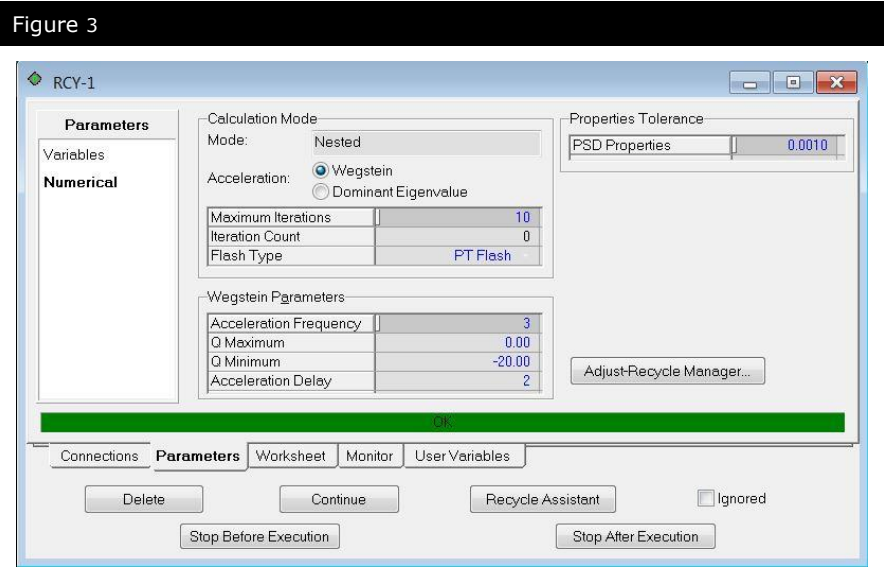
Monitor Tab

This page displays convergence information as the calculations are performed. Any variable that changes between iterations is displayed in this table. In order to view plots of variables as they change during the calculation of the recycle, you must select the variables to view on the **Setup** page.

Worksheet Tab

The Recycle **Worksheet** page displays the Inlet and Outlet stream information. In this instance, notice that the Inlet and Outlet streams have the same values. This is because before we installed the Recycle, the Inlet stream was already calculated by UniSim Design. When the Recycle was connected, the known Inlet conditions were automatically passed to the Outlet stream to serve as the starting guess.

17. Install the second Recycle with the following information:

In this cell...	Enter...
Connections	
Inlet	LD2 Out
Outlet	RCY 2 Out

The final step to solving the flowsheet is to connect the Recycle Outlets as Inlets to Mixer1 and Mixer2. Once this is done, the flowsheet will begin solving.

18. Attach RCY 1 Out as a feed to Mixer 1.

19. Attach RCY 2 Out as a feed to Mixer 2.
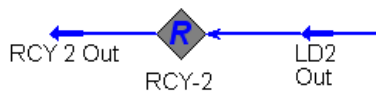
This can be done from the Design tab, Connections page of the Mixers, or from the PFD using attach mode.

Save your case!

Analyzing the Results

Examine the convergence process for the Recycles.

> *Open the Recycle property view and look at the Monitor tab. How many iterations did each Recycle need to converge?*
>
> _____
>
> *Look at the Worksheet tab for each Recycle. How close are the Inlet and Outlet stream variables?*
>
> _____
>
> *Are the vapour fractions identical for the Inlet and Outlet?*
>
> _____

	RCY-1	RCY-2
Inlet Vf		
Outlet Vf		

In the next section you will use the Simulation Balance Tool to examine the simulation results in more detail.

Simulation Balance Tool

The Simulation Balance Tool allows the user to perform overall mass and energy balance checks on their simulation. It can reveal modeling errors even if the simulation appears to be fully converged.

The **Simulation Balance Tool** can be used to:

- Check the mass and energy balances across the entire model or constituent sub-flowsheets or unit operations
- Find hidden errors caused by, for example, convergence failures, numerical tolerances or user input errors

Once run the Simulation Balance Tool also provides an **Overall Mass Balance Monitor** to give a live indication of the status.

Accessing the Simulation Balance Tool

Double-click on the Overall Mass Balance Monitor on the status bar.

There are two ways to access the Simulation Balance Tool:

- From the **Tools** menu, by selecting **Simulation Balance Tool**
- From the **Overall Mass Balance Monitor** on the status bar

Setting the Simulation Balance Tool Parameters

The **Setup** tab is used to set the Simulation Balance Tool tolerances and configuration (Figure 4).

Figure 4
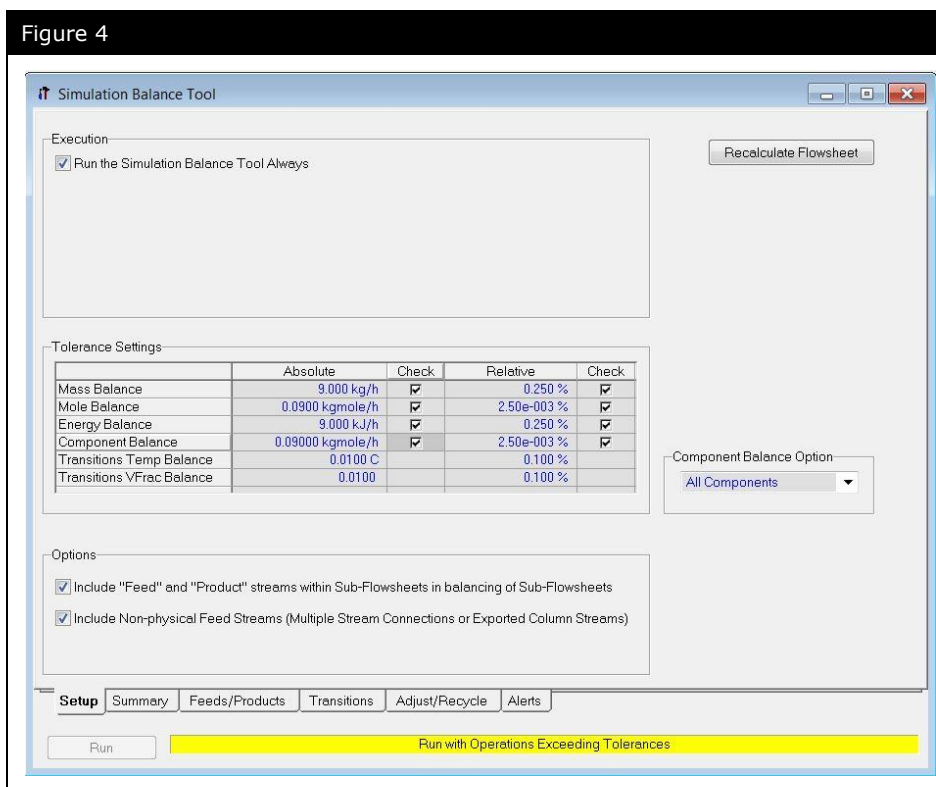
Tolerance Settings

The **Tolerance Settings** are used to specify which balances to perform and the checking tolerance used by the Simulation Balance in the validation.

The **Component Balance Option** group is displayed only when **Component Balance** is checked. This option allows component balances to be performed either for all components or for just a single component.

Configuration Options

The Simulation Balance Tool includes three configuration options controlled by checkboxes:

1. **Run the Simulation Balance Tool Always**

   When this option is checked, the Simulation Balance Tool automatically runs following any change to the flowsheet. If not checked, the Simulation Balance Tool will not recalculate automatically.

2. **Include "Feed" and "Product" streams within Sub-Flowsheets in balancing of Sub-Flowsheets**

   When this option is checked, any feed streams or product streams inside sub-flowsheets which are not connected to streams on the parent flowsheet are taken into consideration when performing the balances for that sub-flowsheet.

3. **Include Non-physical Feed Streams (Multiple Stream Connections or Exported Column Streams)**

   When this option is checked non-physical streams, such as multiple stream connections (single streams connected to multiple unit operations) or exported column streams are properly accounted for by counting each as a separate stream.

Recalculate Flowsheet

The Simulation Balance Tool also includes a command button **Recalculate Flowsheet.** Clicking this button will force UniSim Design to recalculate the entire flowsheet.

Preferences Options

The Simulation Balance Tool setup defaults can be defined in the UniSim Design session Preferences on the **Case Tools** tab, accessed via the **Tools** menu, by selecting **Preferences** (Figure 5).

Figure 5
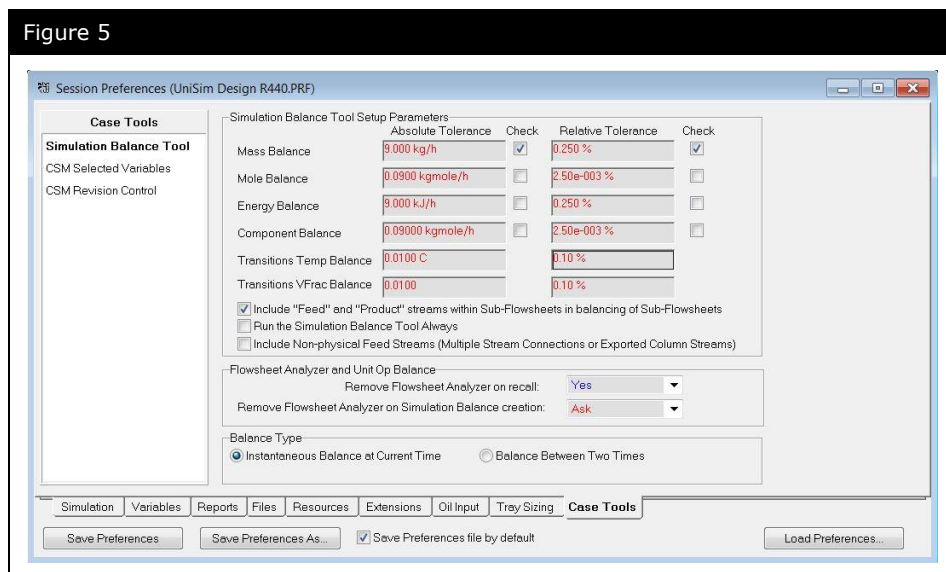
These preferences will apply when a Simulation Balance Tool is first added to a simulation case.

> **Ticking the Run Simulation Balance Tool Always checkbox in the preferences will cause the Simulation Balance Tool to be added to all new cases that are created and also to any old cases that are loaded. It is recommended to make this setting.**

Viewing and Understanding the Simulation Balance Tool Results

Results from the Simulation Balance Tools are reported on five tabs:

Summary Tab – General

The **Summary** Tab, **General** view displays all unit operations where the specified balances exceed the specified tolerances:

Figure 6
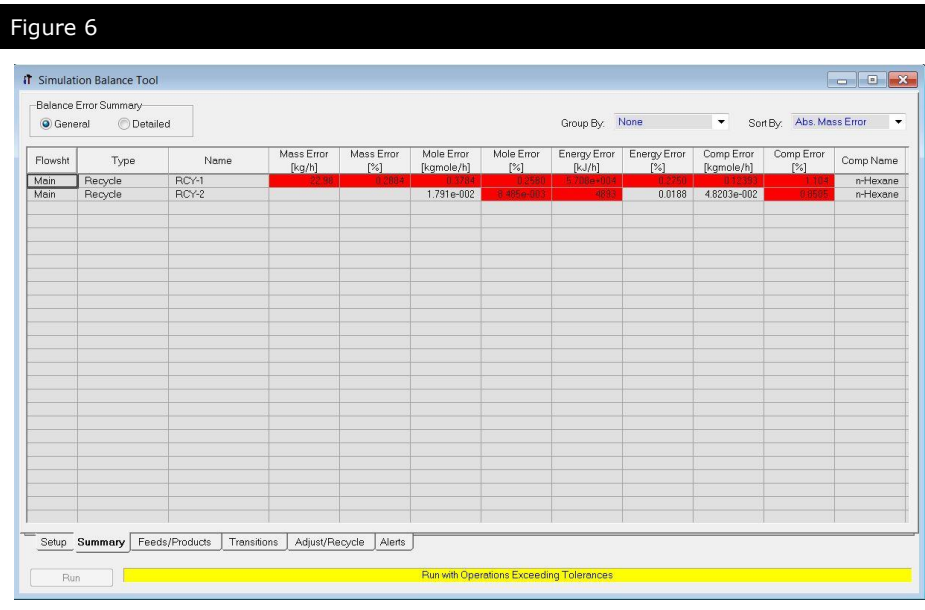
The table gives the following information about the operations:

- **Flowsheet** – the unit operation's parent flowsheet
- **Type** - the UniSim Design object type of the unit operation
- **Name** - the unit operation name. You can double-click on the name to bring up the property view of the unit operation

- **Mass Error** - the mass balance error in both absolute and relative values
- **Mole Error** - the molar balance error in both absolute and relative values
- **Energy Error** - the heat balance error in both absolute and relative values
- **Comp Error** - the component molar balance error in both absolute and relative values
- **Comp Name** - the name of the component with the highest component molar balance error

Cells shown with a red background indicate values which exceed the specified tolerances. Blank cells means the balance error is less than the specified tolerances.

The results can be grouped by **Flowsheet** and **Type** as well as sorted based on the other columns. The grouping and sorting by name is done in ascending order while the rest of the sorting is in descending order.

In Figure 6 the **Summary** tab, **General** view shows a simulation where there are two Recycle unit operations on the Main flowsheet which have errors higher than the specified tolerances. RCY-1 has absolute and relative mass, mole and energy balance errors. RCY-2 has relative mole and absolute energy balance errors.

Summary Tab – Detailed

The **Summary** tab, **Detailed** view gives a unit by unit balance summary in terms of both absolute and relative errors.

Figure 7
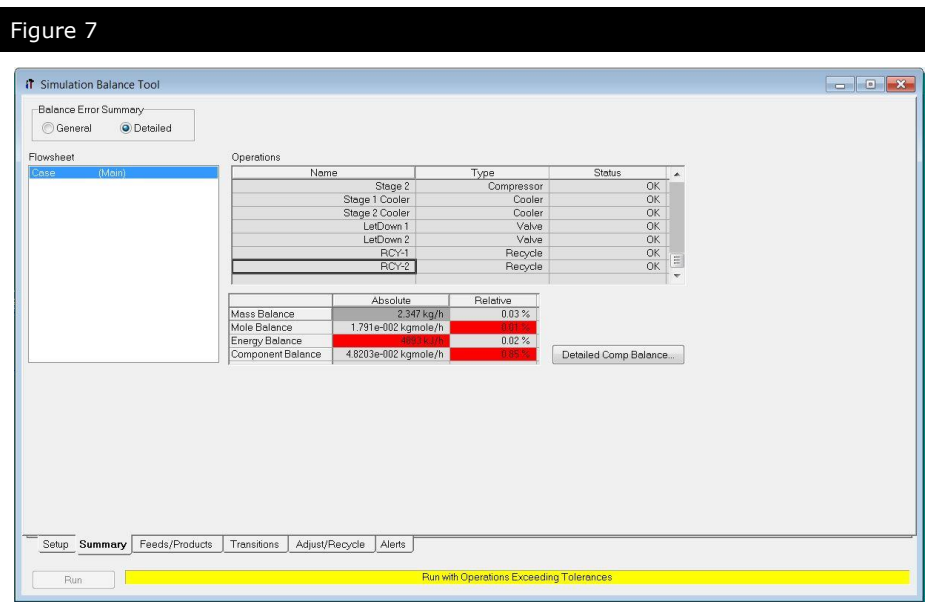
Select the unit operation of interest by selecting the **Flowsheet** containing the unit operation and then clicking the unit operation name under **Operations**.

Double-clicking on the unit operation name will bring up the property view for that unit operation.

Figure 7 shows a simulation where a Recycle unit operation named RCY-2 on the main flowsheet is selected. The detailed balance shows the absolute energy balance error across this operation is 4893 kJ/h. Cells shown with a red background indicate values which exceed the specified tolerances.

Feed/Products Tab

The **Feeds/Products** tab displays the overall mass and energy flows of all the feed and product streams in the simulation, and the overall balance errors.

The **Overall Balance Errors** are displayed using the following color-coding:

- Green - the errors are within the specified tolerances
- Red - the errors exceed the specified tolerances

Figure 8
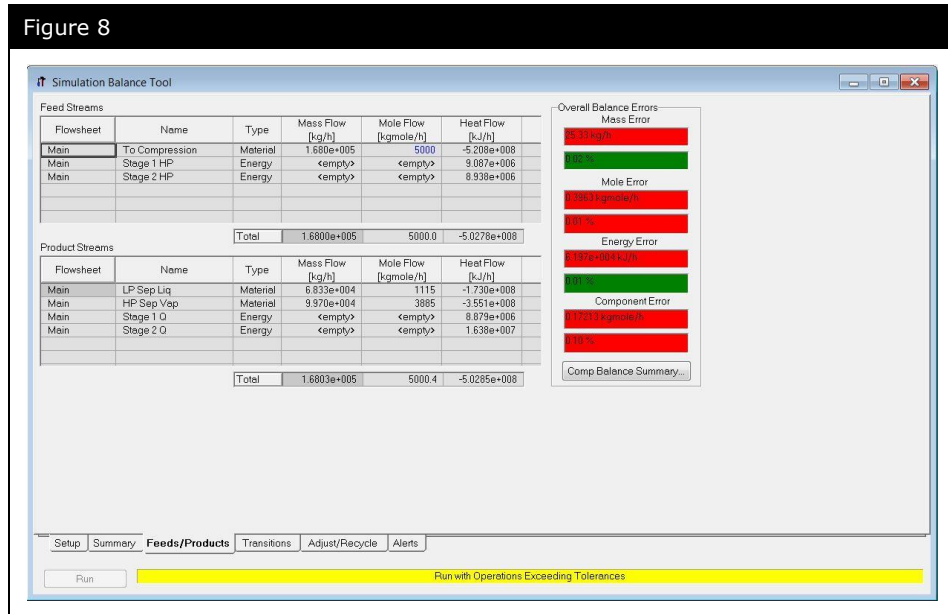
Figure 8 shows a simulation where there are overall mole and component mole balance errors higher than the tolerance on both an absolute and relative basis. The absolute mass balance and absolute energy balance errors are also outside their defined tolerances.

Transitions tab

The **Transitions** tab shows all Transition objects with balance errors larger than the specified tolerances. Transition objects include recycle unit operations, flowsheet boundaries and stream cutters.

Figure 9
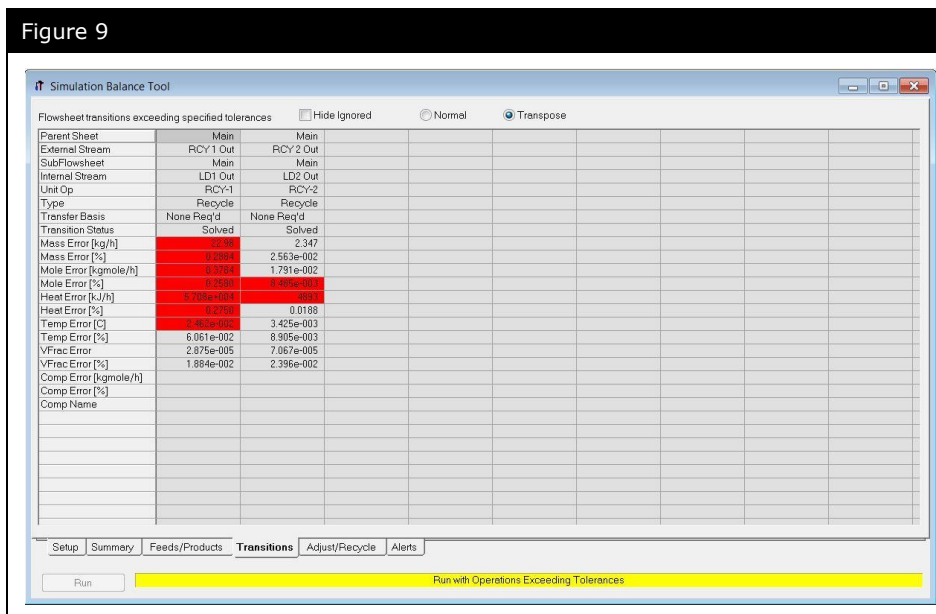
The results can be displayed with the Transitions objects listed by row (**Normal**) or by column (**Transpose**)

Figure 9 shows the **Transitions** tab from a simulation where there are two Recycle unit operations in the Main flowsheet which have errors higher than the specified tolerances.

Adjust/Recycle Tab

The **Adjust/Recycle** tab lists all Adjust and Recycle unit operations in the simulation with their key parameters.

Figure 10
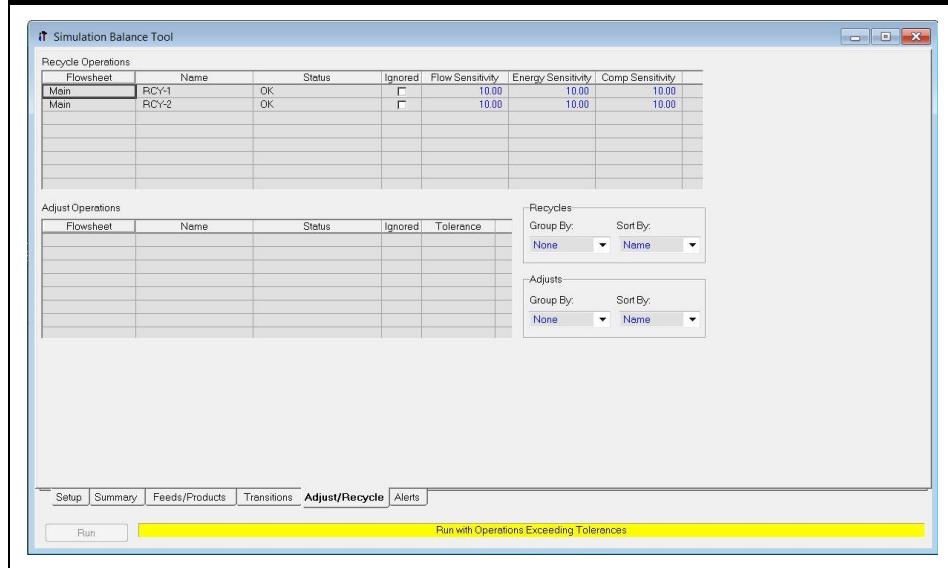
Figure 10 shows the **Adjust/Recycle** tab from a simulation with two Recycle unit operations.

Alerts tab

The **Alerts** tab lists all unit operations in the simulation which have warning or error status messages:

Figure 11
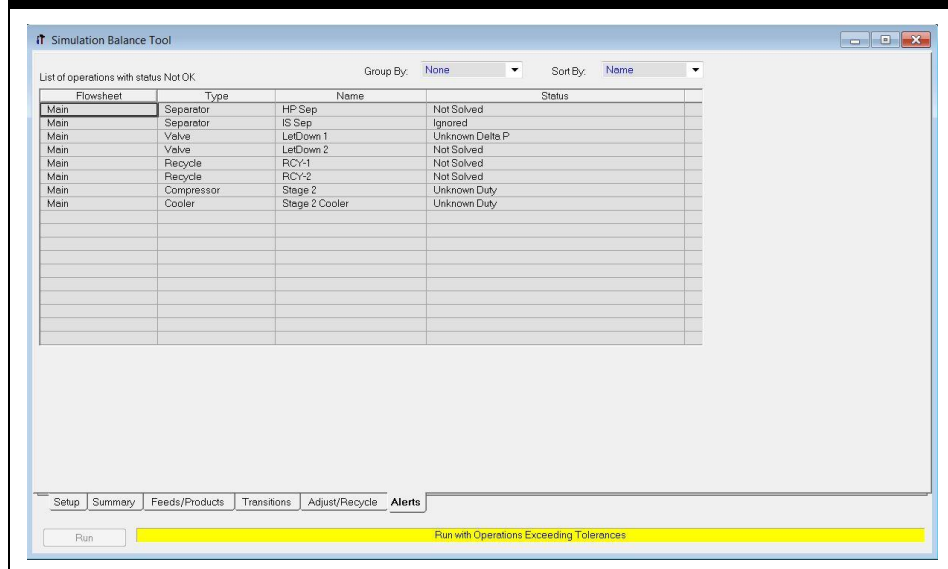
Figure 11 shows the **Alerts** tab from a simulation with eight alert messages, two from separators, two from valves, two from recycle unit operations, one from a compressor and one from a cooler.

Overall Mass Balance Monitor

The **Overall Mass Balance Monitor** provides a live check of the Simulation Balance Tool status. It has four possible values:

- **Balance Tool** – indicating the Simulation Balance Tool has not been run (Figure 12):
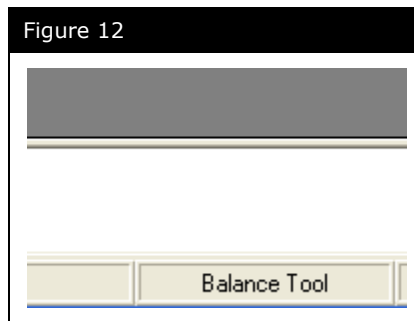
Figure 12

- **Balance Needs Re-running** – indicating the Simulation Balance Tool needs re-running following some change to the flowsheet (Figure 13):
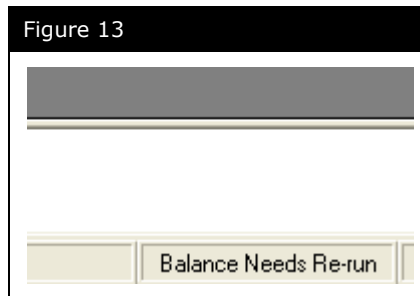
Figure 13

- **Mass Balanced** – indicating the overall mass balance is satisfied to within the tolerances specified by the user (Figure 14):
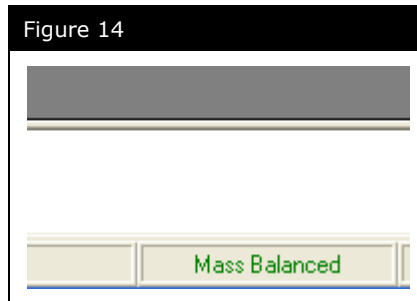
Figure 14

- **Mass Not Balanced** – indicating the overall mass balance is outside the tolerances specified by the user (Figure 15):

Figure 15
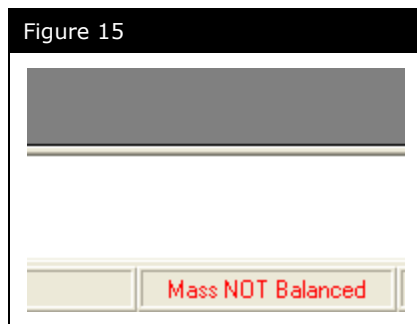
Workshop

The Simulation Balance Tool provides a mechanism to check for material and energy balances within UniSim Design flowsheets as a means to gain a rapid overview of all entities which could be the source of a flowsheeting error even if a flowsheet has a status of converged.

In this workshop you will use the Simulation Balance Tool to check the results of the simulation you built at the beginning of this module.

1. Open the case you saved at the end of the last section (4526.06.TwoStageCompression.usc)

2. From the **Tools** menu, select **Simulation Balance Tool**

3. On the **Setup** tab, enable the mass, mole, energy and component balances with the tolerances as shown in Figure 16:
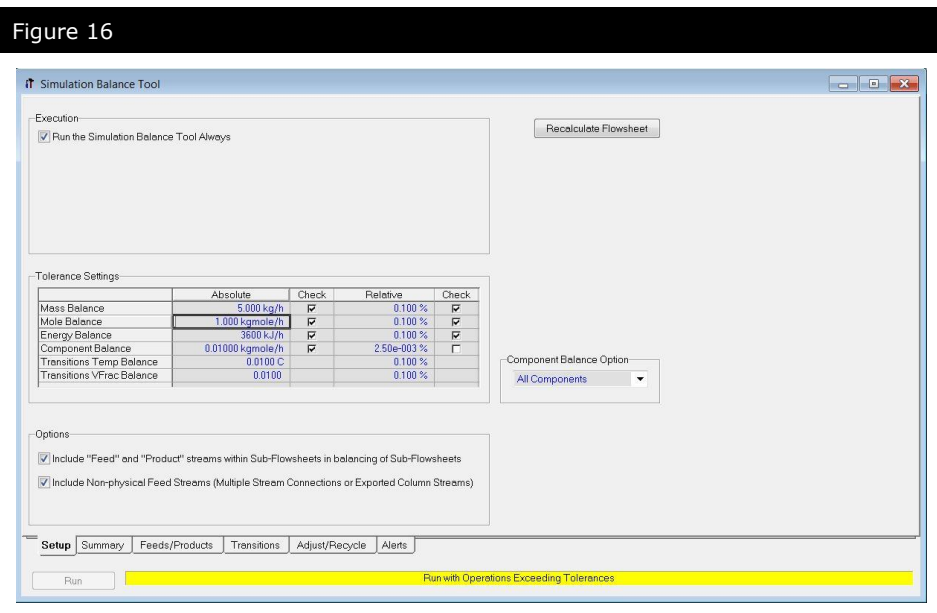
Figure 16

4. Investigate the results of the Simulation Balance Tool using the **Summary, Feeds/Products**, **Transitions**, **Adjust/Recycle** and **Alerts** tabs

---

Are there any unit operations with balance errors? Which ones?
_____

Why do you think these unit operations have balance errors?
_____

Can you think of a way to reduce the errors?
_____

---

5. Go to the **Adjust/Recycle** tab
6. Change the **Comp Sensitivity** for all Recycle unit operations in your model to 0.1
7. Investigate the results of the Simulation Balance Tool using the **Summary**, **Feeds/Products**, **Transitions**, **Adjust/Recycle** and **Alerts** tabs

---

Did reducing the sensitivity resolve the balance errors?
_____

How did it achieve this?
_____

Save your case!

Pipe Segment

The pipe segment is used to simulate a wide variety of piping situations ranging from single or multi-phase plant piping with rigorous heat transfer estimation, to large capacity looped pipeline problems. It offers the common pressure drop correlations developed by Gregory, Aziz, and Mandhane, and Beggs and Brill. A third option, OLGAS, is also available as a gradient method. In addition there are a large number of speciality pressure drop correlations available. Consult the On-line Help and the Manual for more information on these methods. Four levels of complexity in heat transfer estimation allow you to find a solution as rigorously as required while allowing for quick generalized solutions to well-known problems.

The pipe segment offers four calculation modes:

- Pressure Drop
- Length
- Flow
- Diameter

The appropriate mode will automatically be selected depending on the information supplied. In order to solve the pipe, you must supply enough information to completely define both the material balance and the energy balance.

Pipe segments that traverse undulating terrain are subdivided further into a number of segments with elevation points assigned at locations where there is a significant slope change.

Adding a Pipe Segment

In this simulation, we will be using one individual pipe segment operation in the gathering system. In addition, the Pipe operation will contain multiple segments to represent the various elevation rises and drops.

Schedule 40 steel pipe is used throughout and the pipe is buried at a depth of 1 m (3 ft). All pipes are uninsulated.

1. Double-click on the **Pipe Segment** icon from the Object Palette.

Pipe Segment icon

Design tab - Connections page

On the **Connections** page, the Inlet (Feed), Product, and Outlet (Energy) stream connections are made.

2. Complete the **Connections** page as shown below:

Figure 17
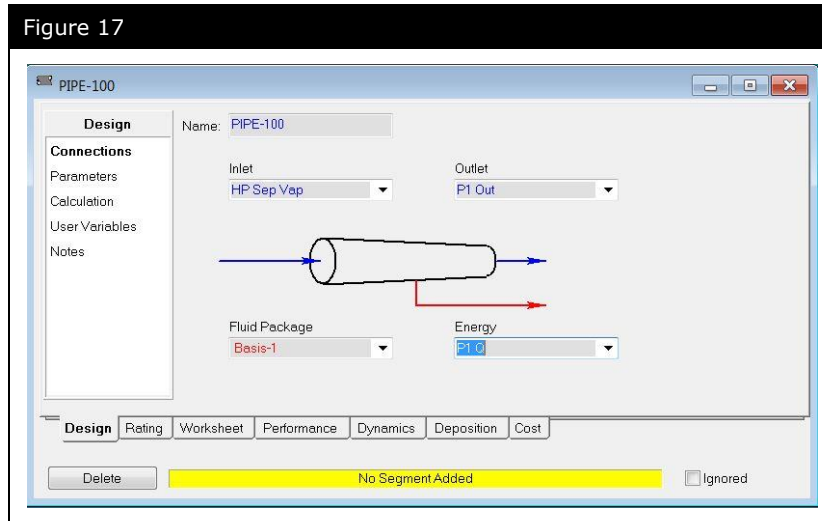
Design tab - Parameters page

On this page, you can select the **Pipe Flow Correlation** which will be used for two-phase (VL) flow calculations. The options are:

- Aziz, Govier & Fogarasi
- Baxendell & Thomas
- Beggs & Brill
- Duns & Ros
- Gregory, Aziz, Mandhane
- Hagedorn & Brown
- OLGAS2000_2P
- OLGAS2000_3P
- Orkiszewski
- Poettman & Carpenter
- Slurry Pipe Correlation
- Tulsa99
- UniSim, Liquid Slip
- UniSim, Homogeneous Flow

For single phase streams, the Darcy equation is used for pressure drop predictions, regardless of the correlation selected on the **Parameters** page. The Darcy equation is a modified form of the mechanical energy equation, which takes into account losses due to frictional effects as well as changes in potential energy.

Additional licenses are required to access the OLGAS correlations. These use 3rd party correlations from SPT Group.

3. In this example the flow through the pipe is single phase vapour so the Darcy equation will be used, hence leave the selected **Pipe Flow Correlation** as **Beggs and Brill** which is the default. If required the pressure drop for the pipe can be supplied on the **Parameters** page. In this example, it will be left empty and calculated.

Rating tab - Sizing page

On the **Sizing** page, you construct the length-elevation profile for the Pipe Segment. Each pipe section and fitting is labeled as a segment. To fully define the pipe section segments, you must also specify pipe schedule, diameter, material and # of increments.

Horizontal pipe sections have an Elevation of 0. Positive elevation indicates that the outlet is higher than the inlet.

PIPE-100 is broken into three segments.

4. Add the first segment to the pipe unit operation by clicking the **Append** button. Specify the following information for the segment:

In this cell...	Enter...
Fitting/Pipe	Pipe
Length	1021 m (3350 ft)
Elevation Change	0 m (0 ft)

5. To specify the diameter, click the **View** button.

6. Select **Schedule 40** as the Pipe Schedule.

7. From the **Available Nominal Diameters** group, select 203.2 mm (8 inch) diameter pipe and click the **Specify** button. The Outer and Inner Diameter will be calculated by UniSim Design.

UniSim Design contains a database for three pipe schedules: 40, 80, and 160.

8. Use the default **Pipe Material**, **Mild Steel** and the default **Roughness**, 4.572e-5 m (0.0018 inch). Close the window.

9. Two more segments are needed to complete the pipe branch.

In this cell...	Enter...	Enter...
Segment	2	3
Fitting/Pipe	Pipe	Pipe
Length	700 m (2297 ft)	600 m (1969 ft)
Elevation Change	-5 m (-16.40 ft)	12 m (39.37 ft)
Schedule	40	40
Nominal Diameter	203.2 mm (8 inch)	203.2 mm (8 inch)

When all three segments have been added and defined, the view should look like this:

Figure 18
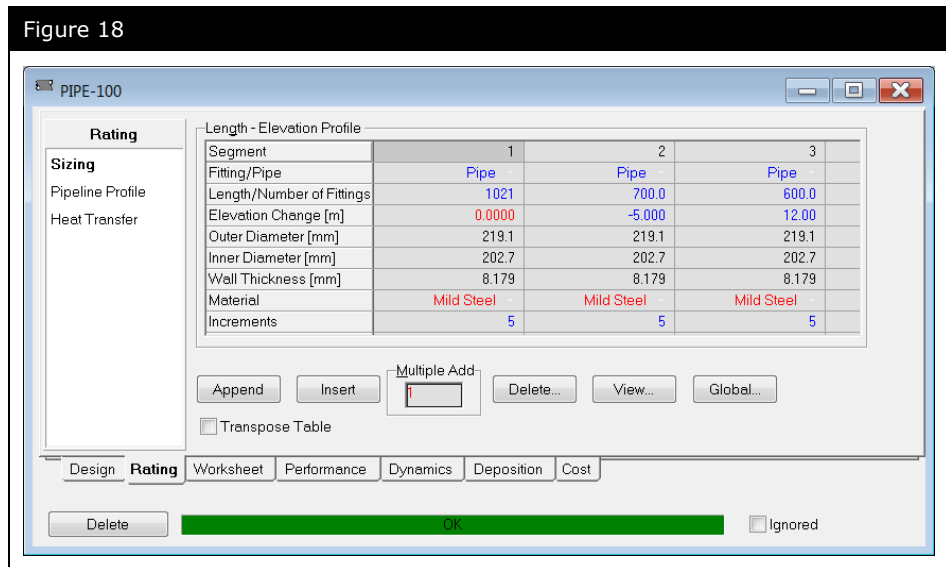
The Pipe segment is able to solve immediately because it defaults to having heat transfer switched off. (None is set as the Heat Transfer Model).

Rating tab - Heat Transfer page

On this page, you select the method that UniSim Design will use for the heat transfer calculations.

The Heat Transfer Model group, at the top of the view, contains three radio buttons. Selecting one of the radio buttons displays one of the three ways of defining heat transfer:

• None (No heat transfer through the pipe wall, considered as an adiabatic pipe)

• Simple (See the details below, this is what this course uses)

• Detailed (The Detailed model allows you to build different wall types and attach them to different segments. Refer to the Operations Guide, section 5.2.3, for more details.)

The following are the valid Heat Transfer combinations for the **Simple model** to solve:

1. Specified Heat Loss value. Enter a Heat Loss value in the Overall Heat Transfer group. No ambient temperature/HTC values should be specified and no options checked on the Estimate HTC page.

2. Overall ambient temperature and HTC. Select the Overall HTC radio button and specify the Overall Ambient Temp and Overall HTC values. No heat loss should be specified and no options checked on the Estimate HTC page.

3. Segment ambient temperatures and HTC. Select the Segment HTC radio button and specify Amb. Temp. and HTC for each segment. No heat loss should be specified and no options checked on the Estimate HTC page.

4. Estimated HTC. Instead of specifying the HTC (per options 2 and 3 above), they can be estimated by checking one or more options on the Estimate HTC page. When estimating HTC, no HTC values should be specified directly; they will be calculated by UniSim Design.

Overall Heat Transfer

If the overall heat duty of the pipe is specified, the heat loss is divided equally between each increment. It is also possible to omit any heat transfer specifications and instead specify both the inlet and outlet temperatures. UniSim Design will assume a linear temperature profile and the overall heat duty will be calculated.

For the pipe in this simulation, we will use the **Simple Heat Transfer Model**, **Segment HTC** and **Estimate HTC** method.

10. On the Rating tab, click on the **Heat Transfer** page.

11. Select the Simple Heat Transfer Model.

12. Select the **Segment HTC** radio button, and enter an Ambient Temperature of **5°C (40°F)** for the first segment.

13. Click on the **Estimate HTC** button, and complete the window that appears as follows:

Figure 19

What is the outlet pressure of PIPE-100?
_____

Pipe Segment Summary

The **Pipeline Profile** page on the **Rating** tab provides a summary table for the segments which make up the Pipe Segment as X,Y coordinates. The distances, length/number of fitting, elevation change, cumulative length and cumulative elevation are displayed for each segment.

Figure 20
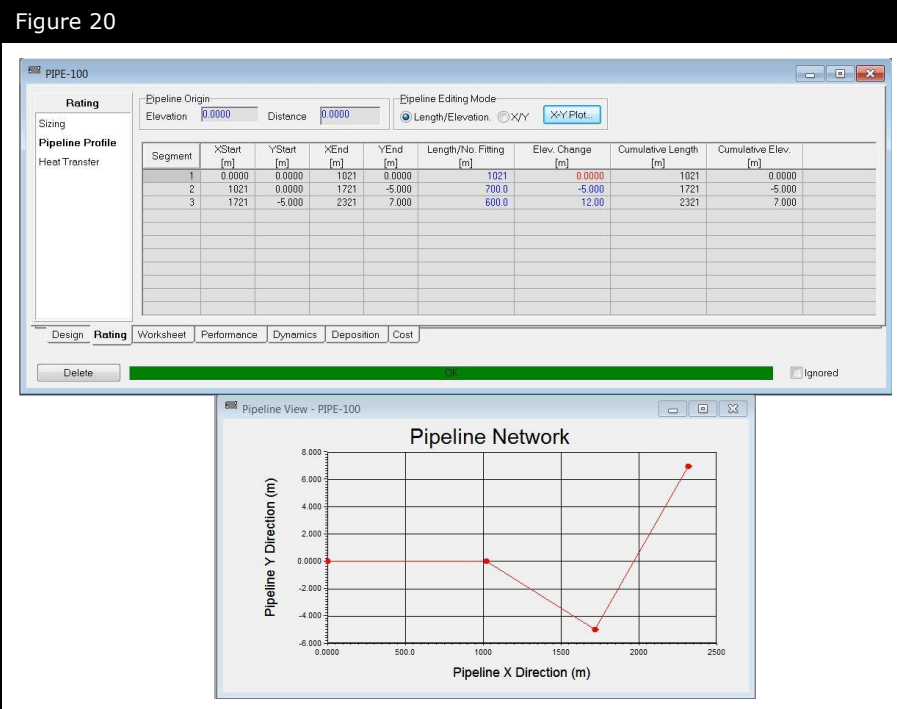
The **Profiles** page on the **Performance** tab provides a summary table for the segments which make up the Pipe Segment. The distance, elevation and number of increments are displayed for each segment.

By clicking the **View Profile** button, you access the **Pipe Profile** view, which consists of a **Table** tab and a **Plot** tab. The **Table** tab shows the following information for each increment along the Pipe Segment:

- Length
- Elevation
- Pressure
- Temperature
- Heat Transferred
- Flow Regime

- Liquid Holdup

- Friction Gradient

- Static Gradient

- Accel Gradient

- Bulk Liquid and Vapor Reynolds Number

- Bulk Liquid and Vapor Velocity

The **Plot** tab graphically displays the profile data that is listed on the **Table** tab. The parameters plotted are selected by radio buttons.

Open the property view for PIPE-100 and examine the **Table** and **Plots** on the **Profiles page** of the **Performance tab**.
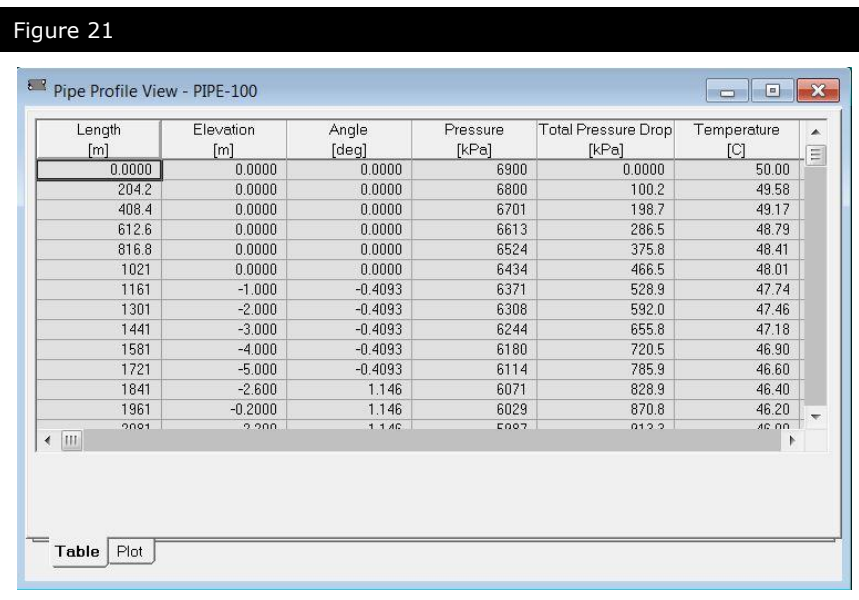
Figure 21

Figure 22
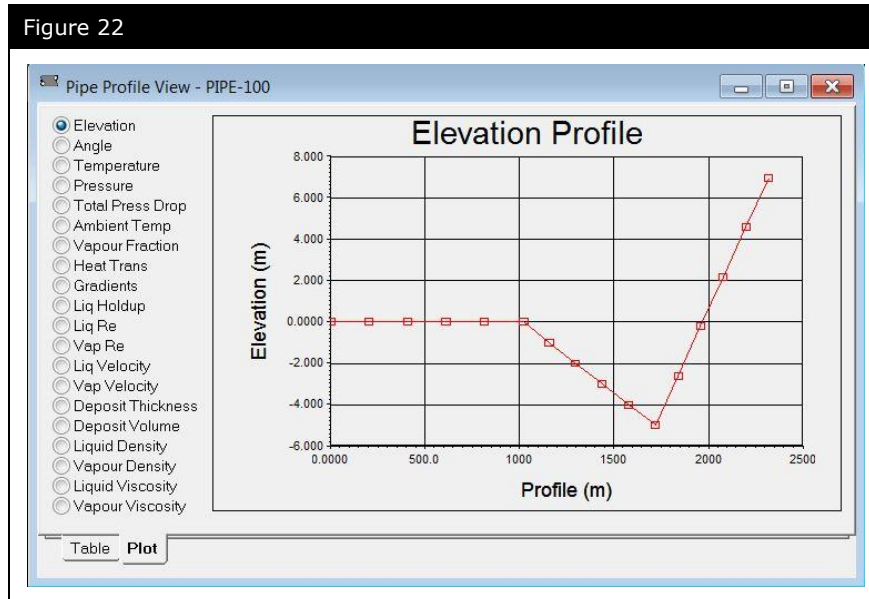
Save your case!

Advanced Modeling

Because the Recycle operation is a mathematical representation of a physical process, its location in a simulation is a particularly important one. The location of the **tear stream** can often determine success or failure to converge a recycle.

Positioning the Recycle Operations for Optimum Performance

When a user is deciding on a tear (Recycle) location, the first choice is often in the actual recycling stream. This is an acceptable choice if only one Recycle operation is being used. However, if more than one block is being used a better location may reduce the calculation time needed to solve the simulation.

Careful choice of recycle position can also reduce the number of Recycle operations that are required. This will reduce the solution time and reduce the number of points at which an error can be introduced if the tolerance is too large.

Try to locate Recycles:

A very poor choice of a tear stream is a stream with an Adjust operation controlling one of its variables.

To define multiple streams (i.e. before Tees, after Mixers). See Answers to the four subsequent Recycle Positioning Exercises are provided at the end of the module in the Answer Key section.

- Exercise 1. This means fewer recycle operations are needed.
- In streams with fixed conditions (i.e. cooler and heater outlets). This means fewer variables need to be iterated on.
- To avoid conflicts with Adjust operations.
- In major flow streams. These are likely to be more stable.

Recycle Positioning Exercises

Answers to the four subsequent Recycle Positioning Exercises are provided at the end of the module in the Answer Key section.

Exercise 1

Examine the following PFD. This flowsheet has three physical recycles and three UniSim Design Recycle operations.

> *What is the minimum number of recycle operations that are needed?*
> _____
>
> *Where should the recycle operation(s) be positioned?*
> _____
> _____

Figure 23 – Exercise 1
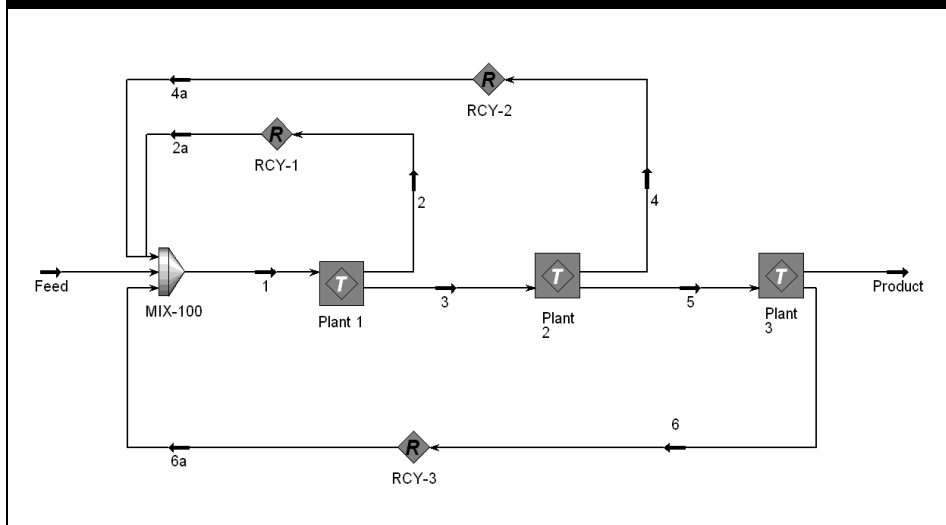
Exercise 2

Assume the condenser outlet stream is fully defined (except flow rate), the chiller duty and outlet conditions are known, the pressure drops across the condenser and chiller are known, and the stage 1 compressor outlet pressure is known.

This flowsheet is the refrigeration loop with economizer from the Challenge at the end of Module 2 of the UniSim Design 4526 course.

How many recycles are needed in this flowsheet, where should they be placed, and why?

_____
_____
_____

Figure 24 – Exercise 2
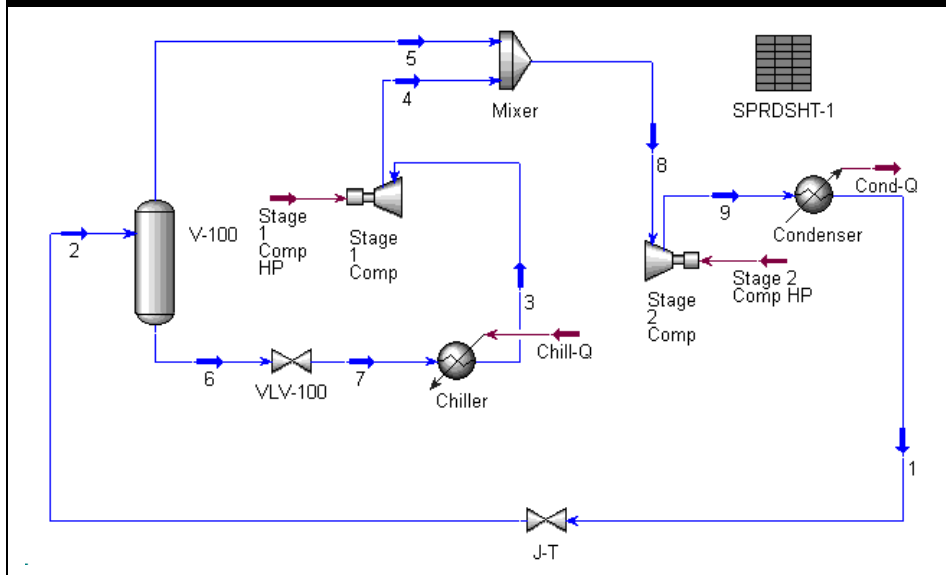
Exercise 3

Assume that the feed stream (To Refrig) is fully defined, all pressure drops are known for the exchanger and the chiller as well as the LTS separator feed temperature.

This flowsheet is the refrigerated gas plant from Module 3 of the UniSim Design 4526 course.

How many recycles are needed in this flowsheet, where should they be placed, and why?

_____

_____

_____

Figure 25 – Exercise 3
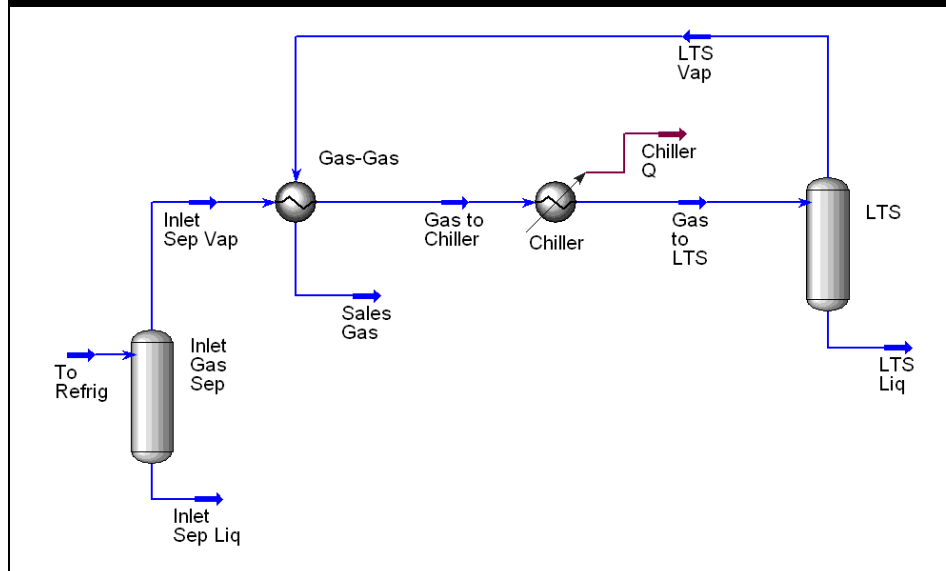
Exercise 4

Assume the Feed is completely defined. Also known are the shell and tube side pressure drops for E-100 and E-101, and the temperatures of streams 3 and 4.

This flowsheet is really an extension of the PFD in Exercise 3. A column and overall material recycle have been appended to the gas plant flowsheet.

> **Note that columns MUST have a fully specified feed stream to solve. (The only exception is that from UniSim Design R380.1 onwards pressure can be propagated backwards from the column to the feed stream).**

> *How many recycles are needed in this flowsheet, where should they be placed, and why?*
>
> _____
>
> _____
>
> _____

Figure 26 – Exercise 4
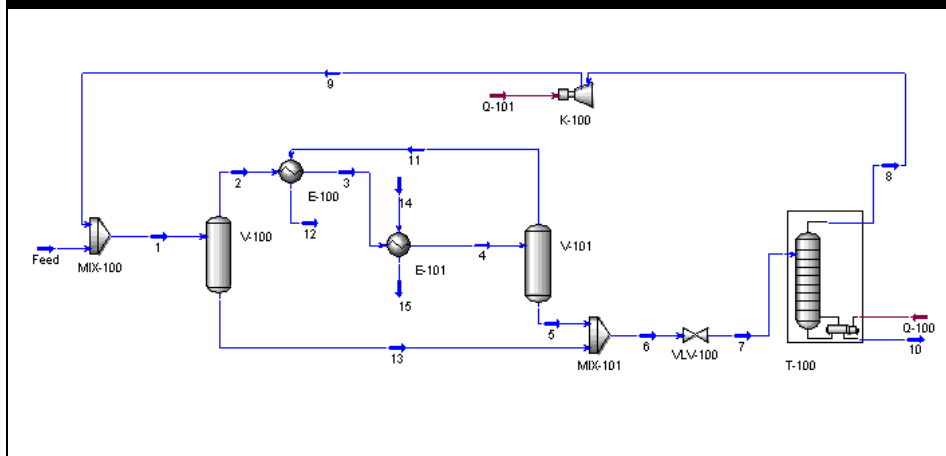
Exercise 5: Compressor Curves

As well as entering curves of head vs flow you can also enter pressure ratio vs flow.

If speed is unknown, you can also estimate the compressor design speed (use the **Design Speed for this Compressor** button on the **Design** tab **Parameters** page). This feature uses a correlation from the GPSA handbook. Consult the UniSim Design **Operations Guide** manual for more details.

After finishing the simulation, your boss provides you with a set of Compressor Curves for the Stage 2 Compressor which now exists in the field. This compressor operates at a speed of 5000 rpm and performs as per the manufacturers curves given below. Will the existing Compressor be able to achieve the outlet pressure you want (i.e. 6900 kPa), or will you have to add a third stage of compression?

Flow, ACT [m3/min (ACFM)]	Head [m (ft)]	Polytropic Efficiency
30 (1000)	6000 (19670)	74
55 (2000)	5950 (19500)	75
95 (3400)	5800 (19000)	75.25
140 (5000)	5500 (18000)	74.5
175 (6200)	4800 (15700)	72
205 (7300)	3360 (11000)	68

Challenge

You complain to your boss that your simulation takes too long to converge on your computer because of the recycles and use this opportunity to petition for a new high speed computer. Your boss has a look at your simulation and denies your request on the basis that you can reduce your convergence time by eliminating one of the recycle unit operations in the simulation. Is your request justified or is your boss correct?

Answer Key

Exercise 1

> **Examine the PFD above. This flowsheet has three physical recycles and three UniSim Design recycle operations. What is the minimum number of recycle operations that are needed?**
>
> *One. There are 3 separate loops and they overlap in stream 1.*
>
> *(Hint. Visualize the separate loops in the system. Which stream is included in all the loops?)*
>
> **Where should the recycle operation(s) be positioned?**
>
> *At the outlet of the mixer.*

Exercise 2

> **How many recycles are needed in this flowsheet, where should they be placed, and why?**
>
> *There is no need for a recycle operation in this refrigeration loop flowsheet due to the positioning of the specifications.*

Exercise 3

> **How many recycles are needed in this flowsheet, where should they be placed, and why?**
>
> *Again there is no need for a recycle operation. Since the LTS separator feed stream has a known temperature and pressure it is fully defined even though the Gas-Gas exchanger hasn't completely solved, hence the separator can solve and then the exchanger can solve.*

Exercise 4

How many recycles are needed in this flowsheet, where should they be placed, and why?

1 recycle needed, 3 possible locations
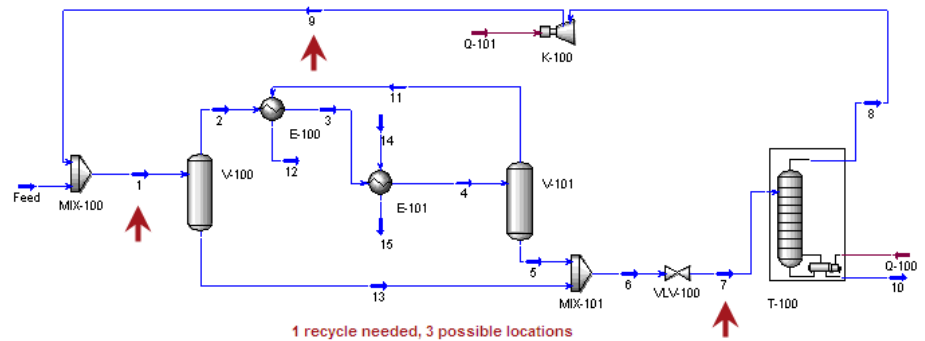
There is no need for a recycle in the small loop containing the two exchangers and separator V-101 because the pressures and temperatures in streams 3 and 4 are known, hence stream 4 can flash fully before the exchangers are solved.

However, the column will not be able to solve unless its feed stream is fully defined, hence a single recycle is needed somewhere in the main loop - for example in stream 1, 7 or 9.

7. Acid Gas Sweetening with DEA

Workshop

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 6900 kPa to 620 kPa before it enters the rich/lean amine exchanger, where it is heated to the regenerator feed temperature of 95°C. The regenerator also consists of 20 real stages. Acid gas is rejected from the regenerator at 50°C, while the lean amine is produced at approximately 110°C. The lean amine is cooled and recycled to the Contactor.

Learning Objectives

Once you have completed this section, you will be able to:

- Simulate Amine towers in UniSim Design
- Supply tray dimensions to calculate component efficiencies for Amine towers
- Use the Set operation
- Use the Spreadsheet

Prerequisites

Before beginning this section you need to be able to start a new case from scratch, add and contact streams and unit operations and be familiar with the column recycle operations.

Process Overview

SET-1

| Multiplier | 1.000 | |
| Increment | -35.00 | kPa |

Makeup H2O

| Temperature | 25.00 | C |
| Comp Mole Frac (H2O) | 1.000000 | |

Cooler

| Pressure Drop | 35.00 | kPa |

MIX-100

| Product Volume Flow | 43.00 | m3/h |
| Equalize Pressures | Yes | |

P-100

| Product Temperature | 35.00 | C |

L/R HEX

Tube Outlet Temperature	95.00	C
Tube Side Pressure Drop	70.00	kPa
Shell Side Pressure Drop	70.00	kPa

VLV-100

| Product Pressure | 620.0 | kPa |

DEA to Contactor

Temperature	35.00	C
Pressure	6865	kPa
Std Ideal Liq Vol Flow	43.00	m3/h
Comp Mass Frac (H2O)	0.718377	
Comp Mass Frac (DEAmine)	0.280090	

Sour Gas

Temperature	25.00	C
Pressure	6900	kPa
Molar Flow	1250	kgmole/h
Comp Mole Frac (Nitrogen)	0.001600	
Comp Mole Frac (H2S)	0.017200	
Comp Mole Frac (CO2)	0.041300	
Comp Mole Frac (Methane)	0.869200	
Comp Mole Frac (Ethane)	0.039300	
Comp Mole Frac (Propane)	0.009300	
Comp Mole Frac (i-Butane)	0.002600	
Comp Mole Frac (n-Butane)	0.002900	
Comp Mole Frac (i-Pentane)	0.001400	
Comp Mole Frac (n-Pentane)	0.001200	
Comp Mole Frac (n-Hexane)	0.001800	
Comp Mole Frac (H2O)	0.012200	
Comp Mole Frac (DEAmine)	0.000000	

Column Overview

Contactor

Figure 1

TS-1		
Current Number of Stages	20	
Top Stage Temperature	35.22	C
Bottom Stage Temperature	56.78	C
Top Stage Pressure	6850	kPa
Bottom Stage Pressure	6900	kPa

Regenerator

Figure 2

Main TS		
Current Number of Stages	18	
Top Stage Temperature	101.6	C
Bottom Stage Temperature	124.4	C
Top Stage Pressure	205.0	kPa
Bottom Stage Pressure	220.0	kPa
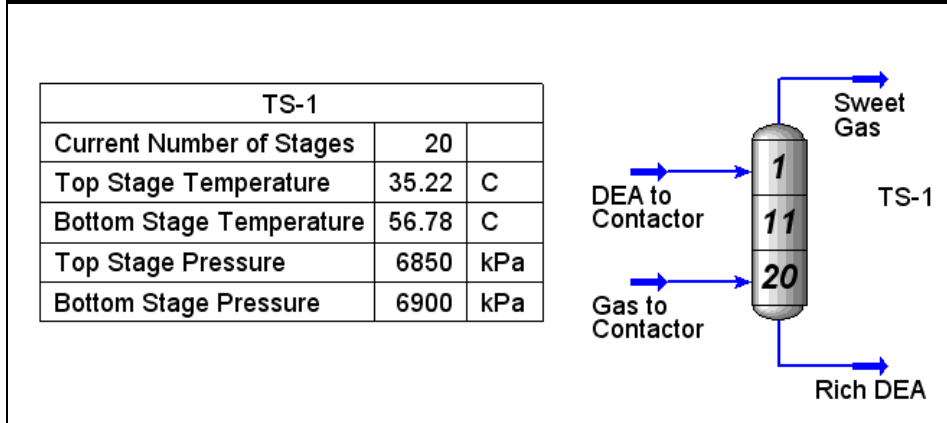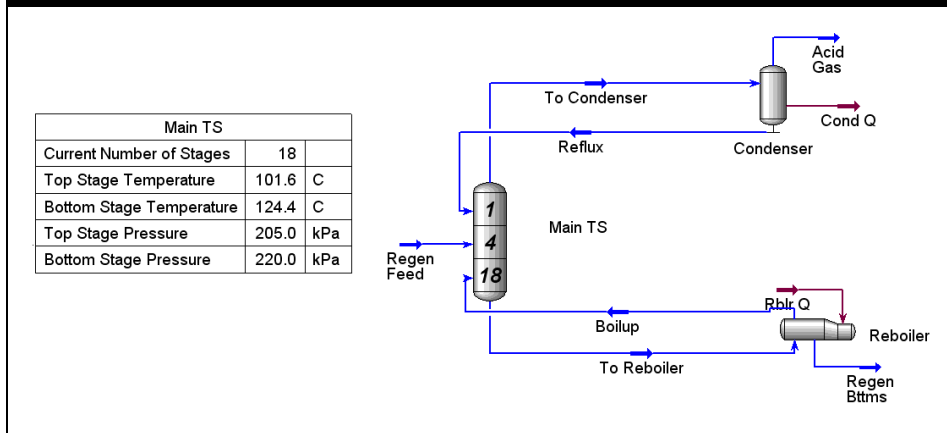
Building the Simulation

Defining the Simulation Basis

The DBRAmine property package does not allow hypothetical components.

For this case, you will be using the DBRAmine property package with the following components:

- Nitrogen
- H2S
- CO2
- Methane
- Ethane
- Propane
- i-Butane

- n-Butane
- i-Pentane
- n-Pentane
- n-Hexane
- H2O
- DEAmine

1. Set up a new case, using the

2. **DBRAmine** property package with the components above. Use the **Kent-Eisenberg** model.

Amines Property Package

You will also find Amine Pkg in the list of Property Packages. This is an older implementation which has been superseded by the DBRAmine package. It is maintained only for compatibility when loading old cases.

The Amines package contains the thermodynamic models developed by D.B. Robinson & Associates for their proprietary amine plant simulator, AMSIM. Their equilibrium acid gas solubility and kinetic parameters for aqueous alkanolamine solutions in contact with H_2S and CO_2 have been incorporated into this property package. The Amines property package has been fitted to extensive experimental data gathered from a combination of D.B. Robinson's in-house data, several unpublished sources and numerous technical references. For more information, refer to Appendix C of the Simulation Basis Manual.

The Amines package incorporates a specialized stage efficiency model to permit the simulation of columns on a real tray basis. The stage efficiency model calculates H_2S and CO_2 component stage efficiencies based on the tray dimensions and the calculated internal tower conditions for both absorbers and strippers.

Adding the Basics

Adding the feed streams

3. Add a new stream for the inlet gas with the following values:

In this cell...	Enter...
Name	Sour Gas
Temperature	25°C (75°F)
Pressure	6900 kPa (1001 psia)
Molar Flow	1250 kgmole/h (25 MMSCFD)
Component	**Mole Fraction**
Nitrogen	0.0016
H2S	0.0172
CO2	0.0413
Methane	0.8692
Ethane	0.0393
Propane	0.0093
i-Butane	0.0026
n-Butane	0.0029
i-Pentane	0.0014
n-Pentane	0.0012
n-Hexane	0.0018
H2O	0.0122
DEAmine	0.0

4. Add a second stream for the lean amine feed to the amine contactor with the following values:

Make sure you enter the DEAmine and H2O compositions on a weight (mass) basis.

In this cell...	Enter...
Name	DEA to Contactor
Temperature	35°C (95°F)
Pressure	6850 kPa (994 psia)
Std Ideal Liq Vol Flow	43 m3/h (190 USGPM)
Component	**Mass Fraction**
H2O	0.72
DEAmine	0.28

The values for the stream DEA to Contactor will be updated once the recycle operation is installed and has calculated.

Adding the Physical Unit Operations

Separator Operation

Any free water carried with the gas is first removed in a Separator operation, FWKO TK.
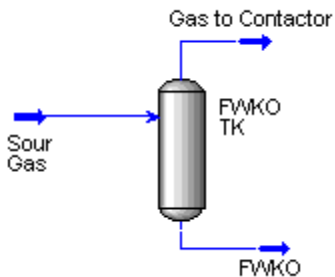
5. Add a Separator and provide the following information:

In this cell...	Enter...
Connections	
Name	FWKO TK
Inlet	Sour Gas
Vapour Outlet	Gas to Contactor
Liquid Outlet	FWKO

What is the flow rate of water in FWKO?

_____

Contactor Operation

The amine contactor is simulated using an Absorber operation in UniSim Design.

6. Add an Absorber column operation with the following specifications:

In this cell...	Enter...
Connections	
Name	DEA Contactor
No. of Stages	20
Top Stage Inlet	DEA to Contactor
Bottom Stage Inlet	Gas to Contactor
Ovhd Vapour Outlet	Sweet Gas

The Input Experts are toggled on and off from the Simulation tab of the Preferences view.

In this cell...	Enter...
Bottoms Liquid Outlet	Rich DEA
Pressures	
Top	6850 kPa (994 psia)
Bottom	6900 kPa (1001 psia)
Estimates	
Top Temperature	40°C (100°F)
Bottom Temperature	70°C (160°F)

The Amines property package requires that real trays be used in the contactor and regenerator operations. To model this in UniSim Design, component specific efficiencies are required for H_2S and CO_2 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. Tray dimensions enable component specific efficiencies to be calculated by estimating height of liquid on the tray and the residence time of vapour in the liquid. To supply the dimensions for Amines calculations, switch to the **Parameters** tab, **Amines** page.

7. Enter the following Tray Section dimensions:

In this cell...	Enter...
Amines	
Weir Height	0.025 m (0.082 ft)
Weir Length	1.0 m (3.3 ft)
Tray Diameter	1.2 m (4.0 ft)

Figure 3
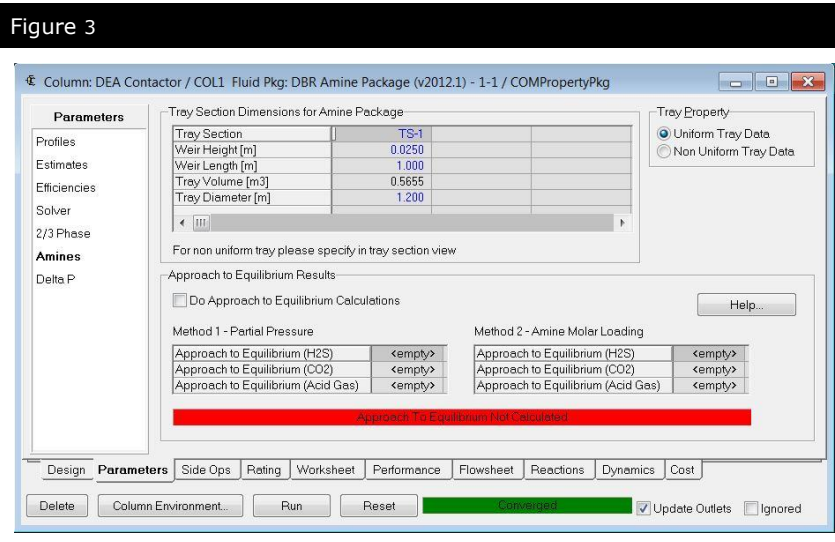
8. **Run** the Column.

9. Once the Column has converged, move to the **Efficiencies** page on the **Parameters** tab.

10. Select the **Component** radio button in the **Efficiency Type** group to view the component efficiencies.

Figure 4
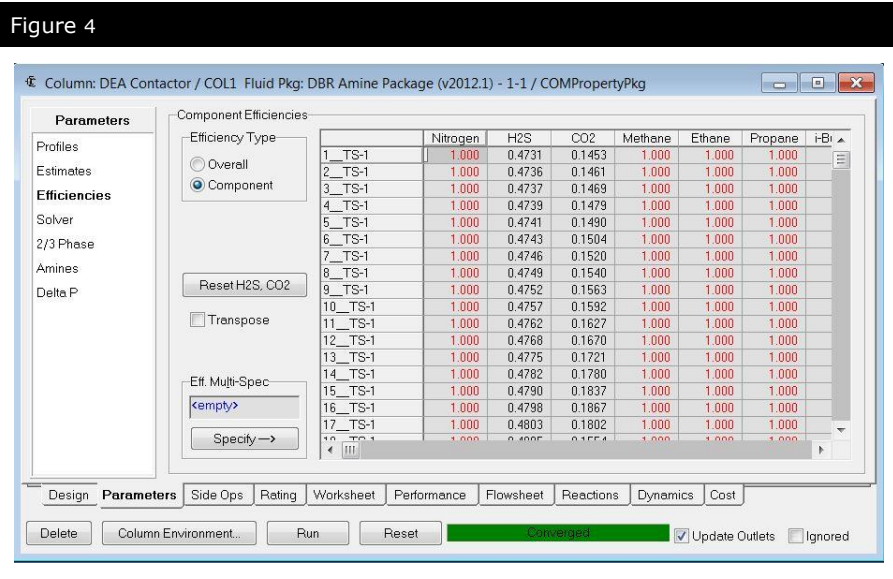
11. Switch to the **Worksheet** tab to view the concentrations of H_2S and CO_2 in the product streams from the column.

What is the concentration of H2S and CO2 in the Sweet Gas?

H2S_____

CO2_____

Valve Operation

Rich DEA from the Contactor is directed to a Valve, VLV-100, where the pressure is reduced to 620 kPa (90 psia), which is close to the Regenerator operating pressure.

12. Add a Valve with the following values:
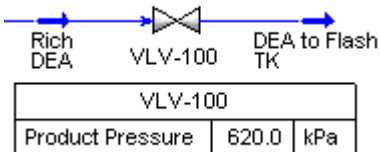
In this cell...	Enter...
Connections	
Inlet	Rich DEA
Outlet	DEA to Flash TK

In this cell...	Enter...
Worksheet	
Pressure, DEA to Flash TK	620 kPa (90 psia)

Separator Operation

Gases which are flashed off from Rich DEA are removed using the rich amine flash tank, Flash TK, which is installed as a Separator operation.

13. Add a Separator with the information shown below:
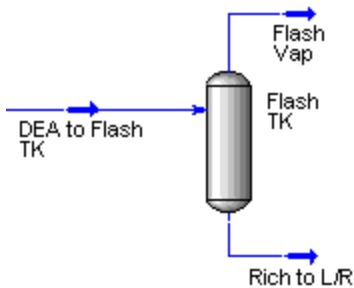
In this cell...	Enter...
Connections	
Name	Flash TK
Inlets	DEA to Flash TK
Vapour Outlet	Flash Vap
Liquid Outlet	Rich to L/R

Heat Exchanger Operation

Regen Feed is heated to 95°C (200°F) in the lean/rich exchanger, L/R HEX, prior to entering the Regenerator, where heat is applied to break the amine-acid gas bonds, thereby permitting the DEA to be recycled to the contactor.

14. Add a Heat Exchanger with the following values:
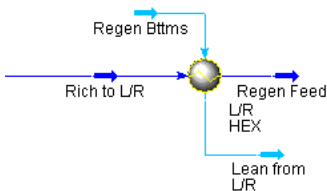
In this cell...	Enter...
Connections	
Name	L/R HEX
Tube Side Inlet	Rich to L/R
Tube Side Outlet	Regen Feed
Shell Side Inlet	Regen Bttms
Shell Side Outlet	Lean from L/R
Parameters	
Tubeside Delta P	70 kPa (10 psi)
Shellside Delta P	70 kPa (10 psi)
Heat Exchanger Model	Exchanger Design (Weighted)
Worksheet	
Regen Feed, Temperature	95°C (203°F)

Regenerator Operation

Damping Factors will have no effect on problems where the heat and spec error does not converge.

Certain columns require the use of a damping factor.

Amine Regenerators, TEG Strippers and Sour Water Strippers use damping factors in the 0.25 – 0.5 range.

The Amine Regenerator is modeled as a Distillation Column. There are 20 real stages - 18 stages in the Tray Section plus a Reboiler and Condenser. The component efficiencies for this tower are assumed to be constant at 0.8 for H_2S and 0.15 for CO_2. The efficiencies of the Condenser and Reboiler must remain at 1.0, so only stages 1-18 should have efficiencies entered for them. A Damping Factor of 0.4 will provide a faster, more stable convergence. The Damping Factor controls the step size used in the outer loop when updating the thermodynamic models in the inner loop.

15. Add a Distillation column with the following information:

In this cell...	Enter...
Design\Connections	
Name	Regenerator
No. of Stages	18
Inlet Streams / Stage	Regen Feed / 4
Condenser Type	Full Reflux
Ovhd Vapour Outlet	Acid Gas
Bottoms Liquid Outlet	Regen Bttms
Reboiler Energy Stream	Rblr Q
Condenser Energy Stream	Cond Q
Parameters\Solver	
Fixed Damping Factor	0.40
Solving Method	Legacy Inside-Out
Parameters\Profiles	
Condenser Pressure	190 kPa (27.5 psia)
Condenser Delta P	15 kPa (2.5 psi)
Reboiler Pressure	220 kPa (31.5 psia)
Top Stage Temperature	100°C (210°F)
Reboiler Temperature	125°C (260°F)
Parameters\Efficiencies	
CO2	0.15
H2S	0.8

You will need to click the **Reset H2S, CO2** button before you can enter the specified H2S and CO2 efficiencies

In this cell...	Enter...
Design\Monitor	
Overhead Vap Rate (Estimate)	75 kgmole/h (1.5 MMSCFD)
Reflux Ratio (Estimate)	1.5
Design\Monitor	
Column Temperature, Condenser	50°C (120°F)
Column Duty, Reboiler	1.3e7 kJ/h (1.2e7 Btu/hr)

Remember to activate the Condenser Temperature and Reboiler Duty specifications once they are added.

An alternative specification that could be used is the Component Recovery for DEA, because all of the DEA (100%) should be recovered in the bottom product stream.

16. **Run** the column.

Mixer Operation

Water make-up is necessary, since water is lost in the Absorber and Regenerator overhead streams. A Mixer operation combines the lean amine from the Regenerator with a water makeup. These streams mix at the same pressure.

The Mixer will adjust the water flow rate to achieve the circulation rate. An Adjust operation could have been used but is not necessary.

17. Add a new stream.

In this cell...	Enter...
Connections	
Name	Makeup H2O
Temperature	25°C (77°F)
Component	**Mole Fraction**
H2O	1.0

18. Add a Mixer with the following information:

In this cell...	Enter...
Connections	
Inlets	Makeup H2O Lean from L/R
Outlet	DEA to Cool
Parameters	
Pressure Assignment	Equalize All
Worksheet	
Std Ideal Liq Vol Flow, DEA to Cool	43 m3/h (190 USGPM)

MIX-100		
Product Volume Flow	43.00	m3/h
Equalize Pressures	Yes	

What is the flow rate of Makeup H2O?
_____

Cooler Operation

19. Add a Cooler with the values given below:
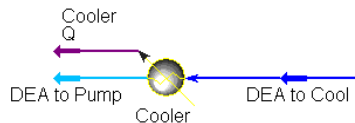
In this cell...	Enter...
Connections	
Name	Cooler
Feed Stream	DEA to Cool
Product Stream	DEA to Pump
Energy Stream	Cooler Q
Parameters	
Pressure Drop	35 kPa (5 psi)

Pump Operation

20. Add a Pump with the following information:
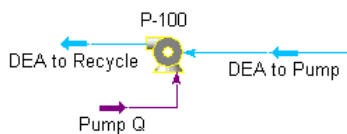
In this cell...	Enter...
Connections	
Inlet	DEA to Pump
Outlet	DEA to Recycle
Energy	Pump Q
Worksheet	
Temperature, DEA to Recycle	35°C (95°F)

Adding Logical Unit Operations

Set Operation

Set icon

The Set is a steady-state operation used to set the value of a specific Process Variable (PV) in relation to another PV. The relationship is between the same PV in two like objects; for instance, the temperature of two streams, or the UA of two exchangers.

21. Double-click on the **Set** icon. Complete the **Connections** tab as shown in the following figure.
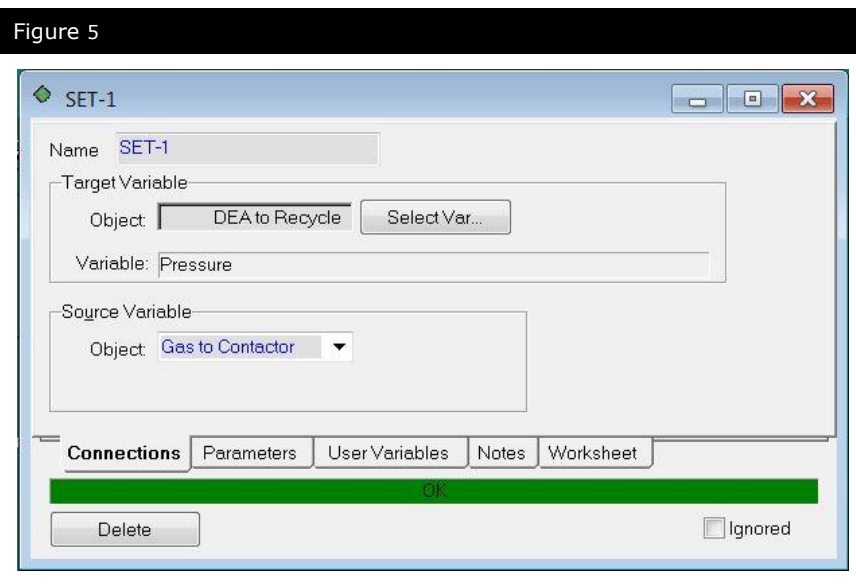
Figure 5

22. Go to the **Parameters** tab. Set the Multiplier to **1,** and the Offset to **-35 kPa** (-5 psi) as shown below:

Figure 6

Recycle Operation

Recycle icon

The Recycle installs a theoretical block in the process stream. The feed into the block is termed the calculated recycle stream, and the product is the assumed recycle stream. The following steps take place during the convergence process:

- UniSim Design uses the conditions of the assumed stream and solves the Flowsheet up to the calculated stream.
- UniSim Design then compares the values of the calculated stream to those of the assumed stream.
- Based on the difference between the values, UniSim Design modifies the values in the assumed stream.
- The calculation process repeats until the values in the calculated stream match those in the assumed stream within specified tolerances.

In this case, the lean amine (DEA to Contactor) stream which was originally estimated will be replaced with the new calculated lean amine (DEA to Recycle) stream and the Contactor and Regenerator will be run until the recycle loop converges.

23. Double-click on the **Recycle** icon. On the **Connections** tab select the connections from the drop-down lists as follows:

Figure 7

24. Switch to the **Parameters** tab. Ensure the tab is as shown in the figure below:
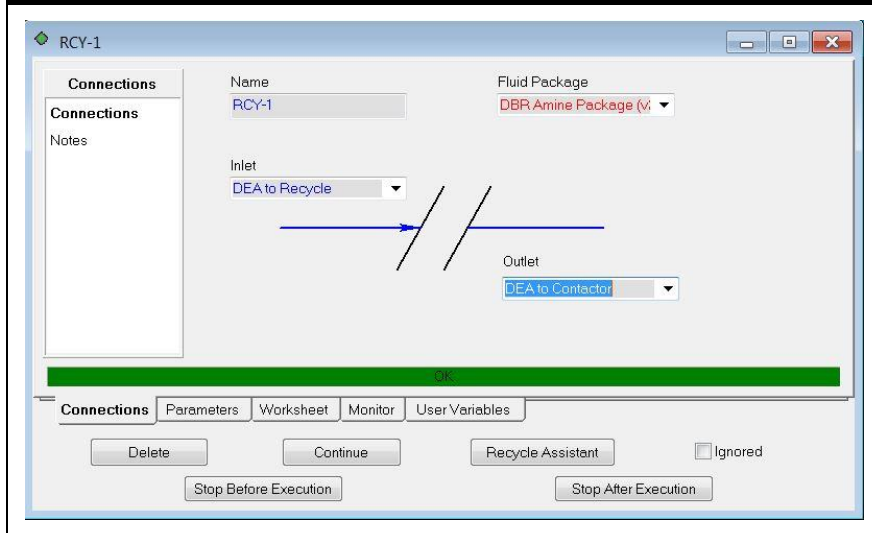
The smaller the Sensitivity the tighter the tolerance.

Figure 8

Save your case!

Analyzing the Results
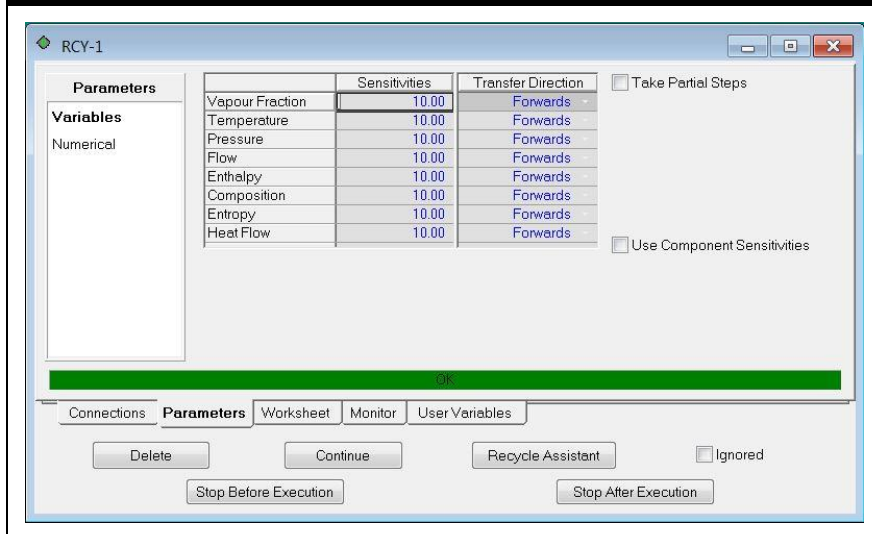
The incoming sour gas contained 4.1% CO_2 and 1.7% H_2S. For our inlet gas flow rate of 1250 kgmole/h (25 MMSCFD), a circulating solution of approximately 28 wt% DEA was used to remove H_2S and CO_2. The conventional pipeline gas specification is no more than 2.0 vol% CO_2 and 4 ppm (volume) H_2S.

To calculate vol ppm multiply liquid volume fraction by 1 million.

What is the C02 vol% in the Sweet Gas?

_____

What is the H2S vol ppm level?

_____

Have the pipeline gas specifications been met?

_____

Advanced Modeling

Concentrations of acid gas components in an amine stream are typically expressed in terms of loadings of amine. Loadings are 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 loadings be directly calculated and displayed, but they can be incorporated into the simulation to provide a "control point" for optimizing the amine simulation.

25. Add a spreadsheet using the following variables for the loading calculations:

Figure 9
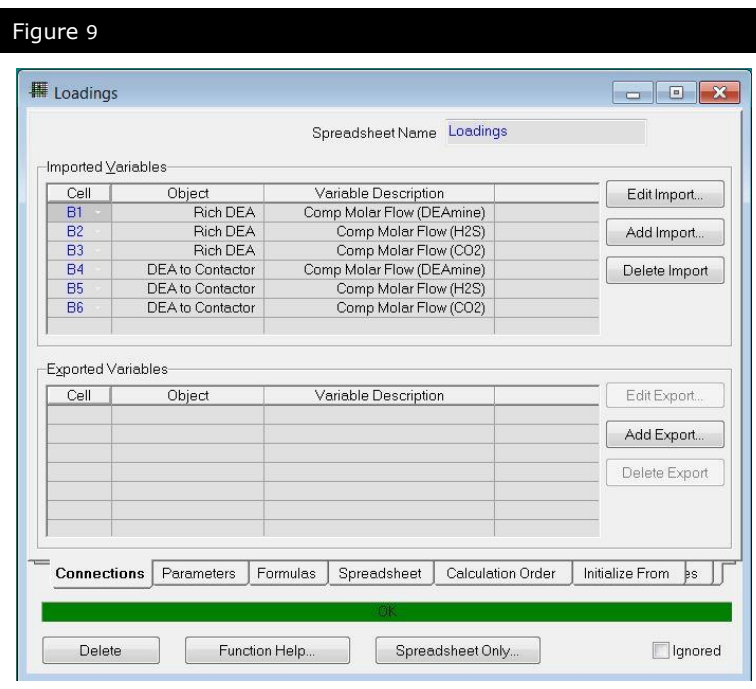
26. On the **Spreadsheet** page, enter the formulae for the loading calculations.

In this cell...	Enter...
Spreadsheet	
D2	=b2/b1
D3	=b3/b1
D5	=b5/b4
D6	=b6/b4

The acid gas loadings can be compared to values recommended by D.B. Robinson.

Maximum Acid Gas Loadings (moles acid gas / moles of amines)		
	CO2	**H2S**
MEA, DEA	0.50	0.35
DEA	0.45	0.30
TEA, MDEA	0.30	0.20

27. Enter appropriate text labels for the imported variables/formulae. Your spreadsheet should appear as shown.

Figure 10
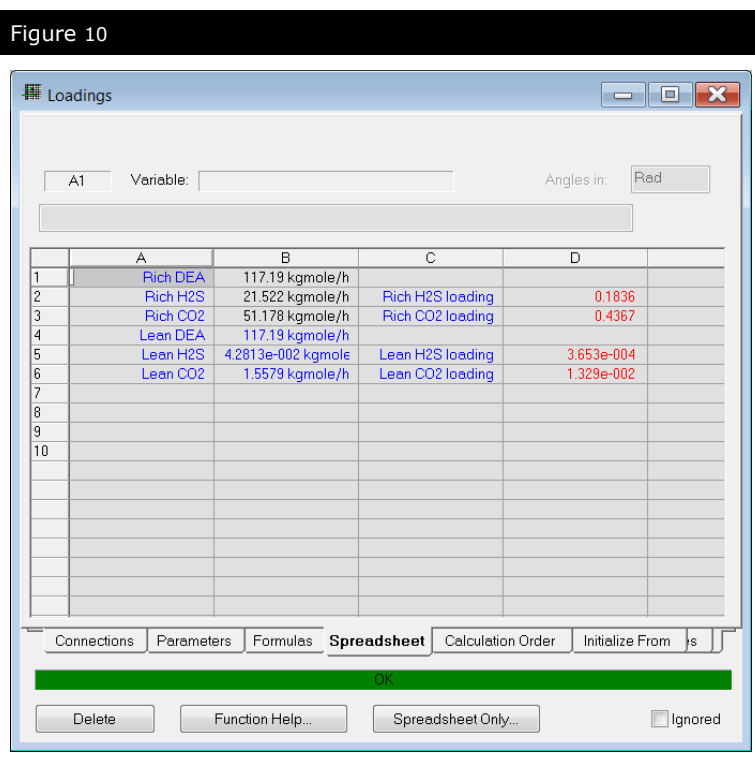
Exploring the Simulation

Exercise 1: Doubling the Flow rate

You just received a phone call from the plant manager at a neighboring gas plant. They are having a problem with their contactor and must shut down. You have agreed to take on their gas for processing, which doubles the flow rate of gas to your plant. Make the necessary changes to handle the upset.

8. Natural Gas Dehydration with TEG

Workshop

At the wellhead, reservoir fluids are generally saturated with water. The water in the gas can present some problems:

- formation of solid hydrates can plug valves, fittings, or pipes
- the presence of water along with H2S or CO2 can cause corrosion problems
- water can condense in the pipeline causing erosion or corrosion problems

Generally, a dehydration unit is used in gas plants to meet a pipeline specification. There are several different processes available for dehydration: glycols, silica gel, or molecular sieves.

The natural gas industry commonly uses tri-ethylene glycol (TEG) for gas dehydration where low gas dew point temperatures are required, such as in the design of offshore platforms in the Arctic or North Sea regions or for other cryogenic processes.

In this example, the water dew point spec for the dry gas is -10°C (-14°F) at 6155 kPa (893 psia).

Learning Objectives

Once you have completed this section, you will be able to:

- Model a typical TEG dehydration unit
- Determine water dew point for a gas

Prerequisites

Before beginning this section you need to be able to add streams, operations and columns.

Process Overview

Inlet Gas		
Temperature	30.00	C
Pressure	6200	kPa
Molar Flow	500.0	kgmole/h
Comp Mass Frac (Nitrogen)	0.001519	
Comp Mass Frac (H2S)	0.028647	
Comp Mass Frac (CO2)	0.067790	
Comp Mass Frac (Methane)	0.782160	
Comp Mass Frac (Ethane)	0.050559	
Comp Mass Frac (Propane)	0.035397	
Comp Mass Frac (i-Butane)	0.018600	
Comp Mass Frac (n-Butane)	0.009458	
Comp Mass Frac (i-Pentane)	0.003913	
Comp Mass Frac (n-Pentane)	0.001957	
Comp Mass Frac (H2O)	0.000000	
Comp Mass Frac (TEGlycol)	0.000000	

Water to Saturate		
Temperature	30.00	C
Pressure	6200	kPa
Molar Flow	0.5000	kgmole/h
Comp Mole Frac (H2O)	1.000000	

RCY-1	
Flow Sensitivity	1.000
Entropy Sensitivity	10.00
Composition Sensitivity	0.1000

Saturate		
Equalize Pressures	Yes	

E-100		
Tube Outlet Temperature	50.00	C
Tube Side Pressure Drop	70.00	kPa
Shell Side Pressure Drop	35.00	kPa

P-100		
Product Pressure	6275	kPa

MIX-100		
Product Volume Flow	0.5000	m3/h
Equalize Pressures	Yes	

L/R HEX		
Shell Outlet Temperature	105.0	C
Tube Side Pressure Drop	70.00	kPa
Shell Side Pressure Drop	70.00	kPa

Column Overview

TEG Contactor
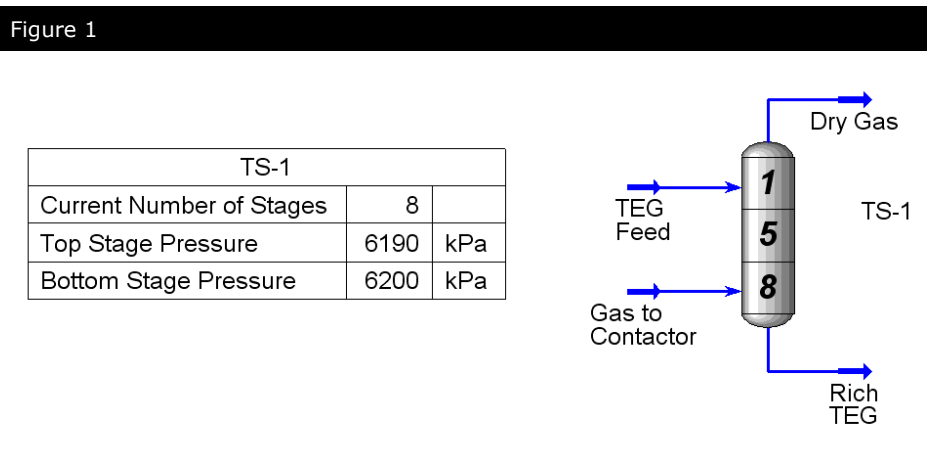
Figure 1

TS-1		
Current Number of Stages	8	
Top Stage Pressure	6190	kPa
Bottom Stage Pressure	6200	kPa

TEG Regenerator

Figure 2

Main TS		
Current Number of Stages	1	
Top Stage Pressure	103.0	kPa

Condenser		
Vessel Pressure	101.0	kPa

Reboiler		
Vessel Pressure	103.0	kPa
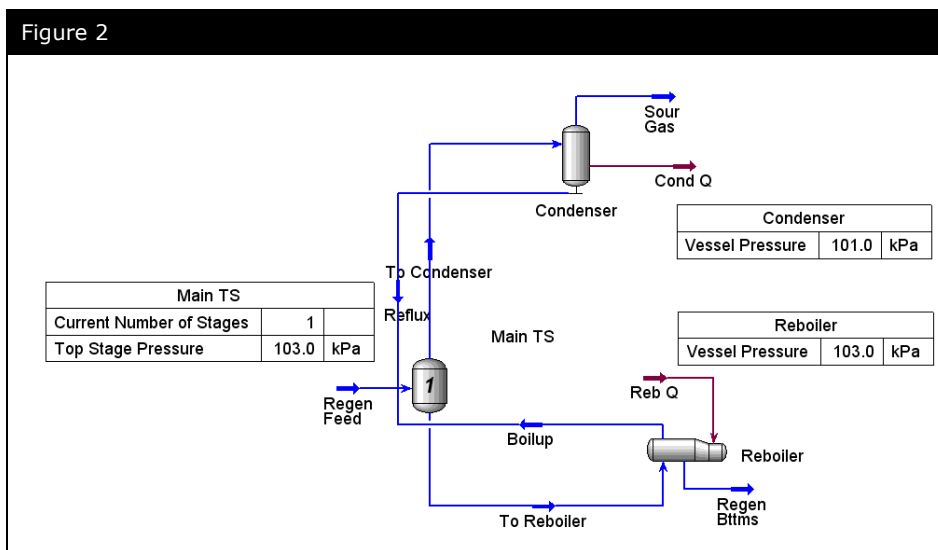
Building the Simulation

Defining the Simulation Basis

For this case, you will be using the **Glycol Package** with the following components:

- Nitrogen
- H2S
- CO2
- Methane
- Ethane
- Propane

- i-Butane
- n-Butane
- i-Pentane
- n-Pentane
- H2O
- TEGlycol

Starting the Simulation

Adding the feed streams

1. Add a Material stream for the inlet gas with the following values:

In this cell...	Enter...
Name	Inlet Gas
Temperature	30°C (85°F)
Pressure	6200 kPa (900 psia)
Molar Flow	500 kgmole/h (10 MMSCFD)
Component	**Mole Fraction**
Nitrogen	0.0010
H2S	0.0155
CO2	0.0284
Methane	0.8989
Ethane	0.0310
Propane	0.0148

In this cell...	Enter...
i-Butane	0.0059
n-Butane	0.0030
i-Pentane	0.0010
n-Pentane	0.0005
H2O	0.0000
TEGlycol	0.0000

2. Add a second Material stream for the TEG feed to the TEG Contactor with the listed values.

In this cell...	Enter...
Name	TEG Feed
Temperature	50°C (120°F)
Pressure	6200 kPa (900 psia)
Std Ideal Liq Vol Flow	0.5 m3/h (2 USGPM)
Component	**Mass Fraction**
H2O	0.01
TEGlycol	0.99

Remember to enter these compositions as mass fractions!

The values for the stream TEG Feed will be updated once the Recycle operation is installed and has calculated.

Mixer Operation

The composition of the natural gas stream has been provided on a water-free basis. To ensure water saturation, the gas is mixed with water prior to entering the Contactor.

3. Add a Mixer to mix the Inlet Gas and Water to Saturate streams.

Saturate	
Equalize Pressures	Yes

Water to Saturate		
Temperature	30.00	C
Pressure	6200	kPa
Molar Flow	**1.0000**	kgmole/h
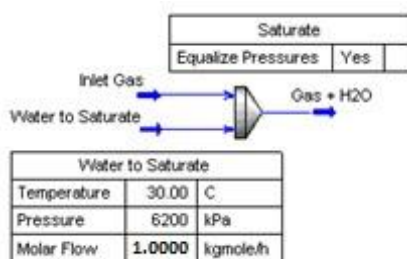
In this cell...	Enter...
Connections	
Name	Saturate
Inlets	Inlet Gas Water to Saturate
Outlet	Gas + H2O
Parameters	
Automatic Pressure Assignment	Equalize All
Worksheet	
Water to Saturate, Flow rate	1 kgmole/h (2.2 lbmole/hr)
Water to Saturate, Composition	100% Water
Water to Saturate, Temperature	30°C (85°F)

What is the vapour fraction of the stream Gas+H20? (It should be less than 1.0 to ensure saturation)

_____

Separator Operation

Any free water carried with the gas is first removed in a separator operation, **FWKO**.

4. Add a Separator and provide the following information:
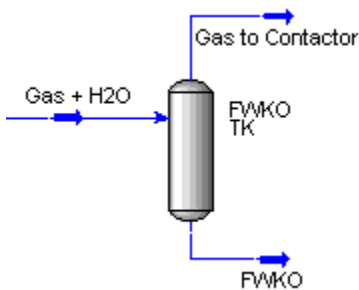
In this cell...	Enter...
Connections	
Name	FWKO TK
Inlets	Gas + H2O
Vapour Outlet	Gas to Contactor
Liquid Outlet	FWKO

How much water is removed by the Separator?

_____

Later in this workshop a hydrate temperature is also calculated for stream Gas to Contactor. At this stage if a Hydrate Formation utility is added to the stream it won't calculate because it does not support the Glycol Package.

Contactor Operation

The TEG Contactor can now be simulated.

5. Add an Absorber column operation with the following specifications and **Run** the column.

In this cell...	Enter...
Connections	
Name	TEG Contactor
No. of Stages	8
Top Stage Inlet	TEG Feed
Bottom Stage Inlet	Gas to Contactor
Ovhd Vapour Outlet	Dry Gas
Bottoms Liquid Outlet	Rich TEG
Pressure	
Top	6190 kPa (897 psia)
Bottom	6200 kPa (900 psia)

Valve Operation

The Rich TEG stream is flashed across the valve, VLV-100. The outlet pressure will be back calculated.

6. Add a Valve with the following values:

In this cell...	Enter...
Connections	
Inlet	Rich TEG
Outlet	LP TEG

Heat Exchanger Operation

Regen Feed is heated to 105°C (220°F) in the lean/rich exchanger, L/R HEX, before entering the Regenerator.

7. Add a Heat Exchanger with the following values:
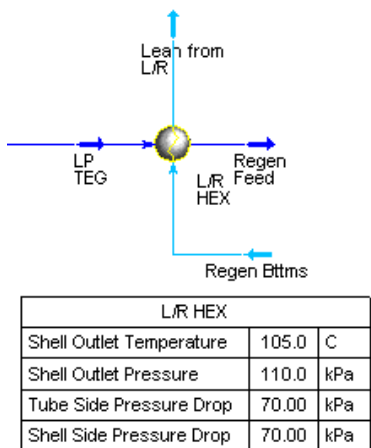
In this cell...	Enter...
Connections	
Name	L/R HEX
Tube Side Inlet	Regen Bttms
Tube Side Outlet	Lean from L/R
Shell Side Inlet	LP TEG
Shell Side Outlet	Regen Feed
Parameters	
Tubeside Delta P	70 kPa (10 psi)
Shellside Delta P	70 kPa (10 psi)
Worksheet	
Regen Feed, Temperature	105°C (220°F)
Regen Feed, Pressure	110 kPa (16 psia)

L/R HEX		
Shell Outlet Temperature	105.0	C
Shell Outlet Pressure	110.0	kPa
Tube Side Pressure Drop	70.00	kPa
Shell Side Pressure Drop	70.00	kPa

Regenerator Operation

The TEG Regenerator is simulated as a Distillation Column. The TEG Regenerator consists of a condenser, a reboiler and one ideal stage.

8. Add a Distillation Column to the case.

You can turn off the Column Input Experts in Tool/Preferences on the Simulation tab by un-checking the 'Use Input Experts' box.

In this cell...	Enter...
Connections	
Name	TEG Regenerator
No. of Stages	1
Inlet Stream	Regen Feed
Condenser Type	Full Reflux
Ovhd Vapour Outlet	Sour Gas
Bottoms Liquid Outlet	Regen Bttms
Condenser Energy Stream	Cond Q
Reboiler Energy Stream	Reb Q
Pressures	
Delta P Cond	2 kPa (1 psia)
Condenser	101 kPa (14 psia)
Specs	
First Spec - Column Temperature	
Stage	Condenser
Spec Value	102°C (215°F)
Status	Active
Second Spec - Column Temperature	
Stage	Reboiler
Spec Value	205°C (400°F)
Status	Active
Third Spec - Reflux Ratio	
Spec Value	1.0 Molar
Status	Estimate
Fourth Spec - Column Draw Rate	
Draw	Sour Gas @ COL2
Spec Value	1 kgmole/h (0.02 MMSCFD)
Status	Estimate

9. Set the **Damping** method (on the **Solver** page of the **Parameters** tab) to **Adaptive**. This will result in much faster convergence for this column.

10. **Run** the Column.

Mixer Operation

TEG is lost in small quantities in the top products of the columns, so a makeup stream is required to ensure that the material balance is maintained.

11. Add a Material Stream with the following information:

Don't forget to enter the compositions as mass fractions!

In this cell...	Enter...
Connections	
Name	Makeup TEG
Temperature	15°C (60°F)
Component	**Mass Fraction**
H2O	0.01
TEG	0.99

12. Add a Mixer with the following information:
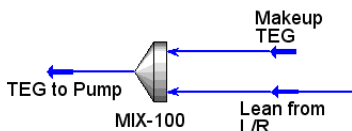
MIX-100		
Equalize Pressures	Yes	
Product Volume Flow	0.5000	m3/h

In this cell...	Enter...
Connections	
Inlets	Makeup TEG Lean from L/R
Outlet	TEG to Pump
Parameters	
Automatic Pressure Assignment	Equalize All
Worksheet	
Std Ideal Liq Vol Flow, TEG to Pump	0.5 m3/h (2 USGPM)

What is the flow rate of Makeup TEG?

_____

Pump Operation

A pump is installed to raise the pressure of the TEG before it enters the Contactor.

13. Add a Pump with the following information:
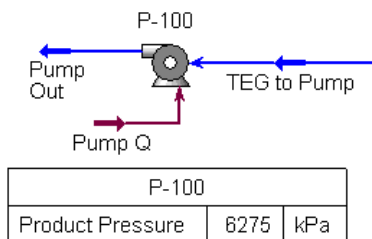
In this cell...	Enter...
Connections	
Inlet	TEG to Pump
Outlet	Pump Out
Energy	Pump Q
Worksheet	
Pump Out, Pressure	6275 kPa (910 psia)

Heat Exchanger

A second heat exchanger is added to cool the TEG returning to the Contactor.

14. Add a Heat Exchanger with the following information:
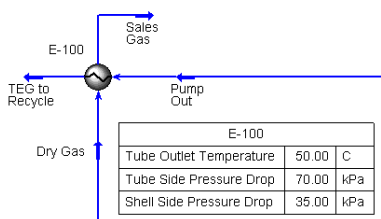
In this cell...	Enter...
Connections	
Tube Side Inlet	Pump Out
Tube Side Outlet	TEG to Recycle
Shell Side Inlet	Dry Gas
Shell Side Outlet	Sales Gas
Parameters	
Tube Side Delta P	70 kPa (10 psi)
Shell Side Delta P	35 kPa (5 psi)
Worksheet	
TEG to Recycle, Temperature	50°C (120°F)

Recycle Operation

Recycle icon

The Recycle installs a theoretical block in the process stream. The feed into the block is termed the calculated recycle stream, and the product is the assumed recycle stream. The following steps take place during the convergence process:

- UniSim Design uses the conditions of the assumed stream and solves the Flowsheet up to the calculated stream
- UniSim Design then compares the values of the calculated stream to those of the assumed stream
- Based on the difference between the values, UniSim Design modifies the values in the assumed stream
- The calculation process repeats until the values in the calculated stream match those in the assumed stream within specified tolerances

The specifications in the lean TEG (TEG Feed) stream which were originally estimated will be replaced by values updated by the recycle. The recycle will control iterations of the loop until it converges.

15. Double-click the **Recycle** icon from the Object Palette. On the **Connections** tab select the connections from the drop-down boxes as depicted below:
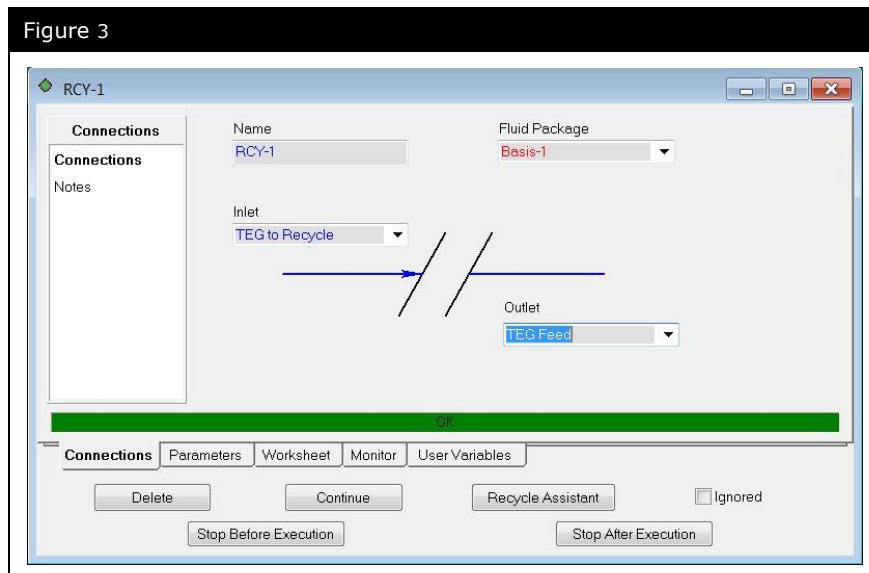
Figure 3

16. Switch to the **Variables** page on the **Parameters** tab. Complete the page as shown in the figure below. Tolerances for **Flow**, **Enthalpy** and **Composition** need to be tightened.

Figure 4
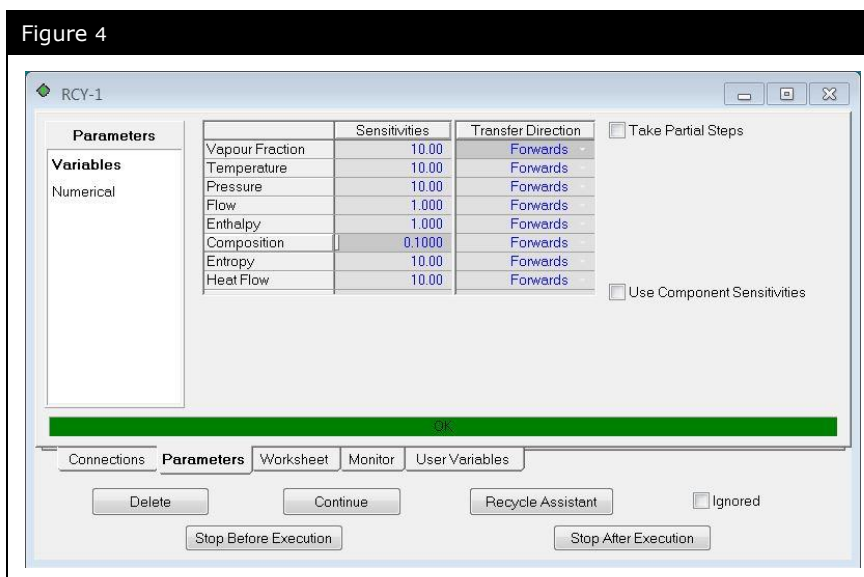
The TEG concentration is very high so it is necessary to tighten the tolerances, especially for composition, to ensure an accurate solution.

Remember to answer NO to the question: "Do you want to return to the simulation environment in HOLDING mode".

Hydrate Formation Utility

1. The Hydrate Formation Utility does not support the Glycol Package. Therefore, in order to use the utility, we need to make a copy of the process stream and edit that stream to use a different fluid package (Peng Robinson).

2. Navigate to the Basis Environment, and use the Copy button the Fluid Pkgs tab. Once copied, open the new fluid package and change the Property Package Selection from Glycol Pkg to **Peng Robinson**".

3. Change the name of the original fluid package from Basis-1 to Glycol, and the new fluid package from Basis-2 to PR. Return to the Simulation Environment.

4. Add a new stream called Gas to **Contactor-2**. Use the Define From Other Stream button to define this stream from the original Gas to Contactor stream.

5. On the Worksheet tab, Conditions page, change the Fluid Package option to **PR**.

6. Repeat steps 4 and 5 to make a second stream, which will be a copy of the **Sales Gas** stream.

Remember to answer NO to the question: "Do you want to return to the simulation environment in HOLDING mode".

Attach a Hydrate Formation Utility to Sales Gas stream

There are three ways to attach utilities to streams.

- Click on the **Tools** menu and select **Utilities**. The **Available Utilities** view appears

- Press **Ctrl U** and the **Available Utilities** view appears

- Double-click a stream. On the **Attachments** tab, select **Utilities**. Click **Create** and the **Available Utilities** view appears

Add a Hydrate Formation Utility.

1. Press **Ctrl U** and in the **Available Utilities** view, select the **Hydrate Formation Utility** and click on the **Add Utility** button. If the utility is not already associated with a stream, then the Hydrate Formation Utility view appears.

2. Click **Select Stream** and select the **Sales Gas**. Click **OK**.

3. Switch to the **Performance** tab. Here you will see the Equilibrium Phase reported as Vapour Phase.

Figure 5
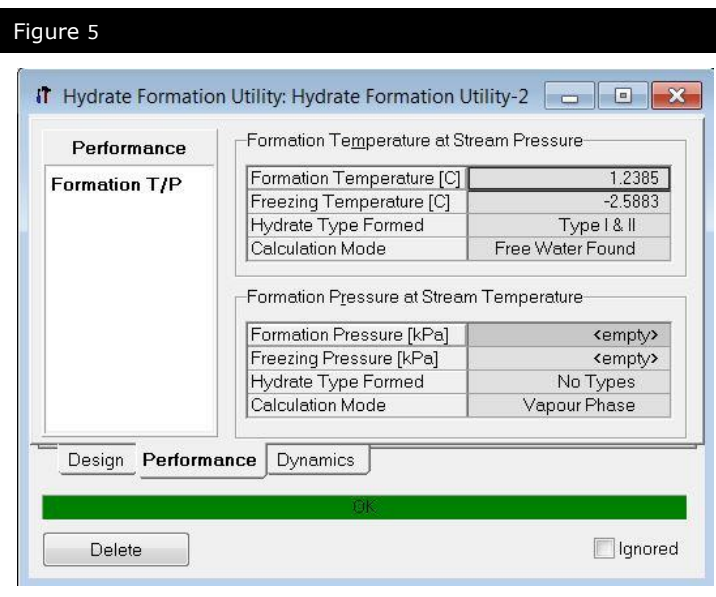
> *What is the hydrate temperature of the Sales Gas stream?*
>
> _____
>
> *How does this compare with the hydrate temperature of the Gas to Contactor stream?*
>
> _____

Save your case!

Analyzing the Results

One of the criteria used to determine the efficiency of a dehydration facility is the water dew point of the dry gas. First, all traces of TEG must be removed from the stream being tested because TEG affects the water dew point. This is accomplished by the use of a Component Splitter. A property correlation is used to calculate the water dew point temperature.

Component Splitter icon

4. Add a Component Splitter with the following values:

In this cell...	Enter...
Connections	
Name	Remove TEG
Inlet	Sales Gas
Overhead Outlet	TEG Only
Bottoms Outlet	Water Dew point
Energy	Split Q
Parameters	
TEG Only, Temperature	35°C (95°F)
Water Dew Point, Temperature	35°C (95°F)
Stream Specifications	Equalize All Stream Pressures
Splits	
Stream TEG Only, TEG	1.0
Stream TEG Only, all other components	0.0

The Component Splitter does not do a flash to separate components. The separation is specified by the user.
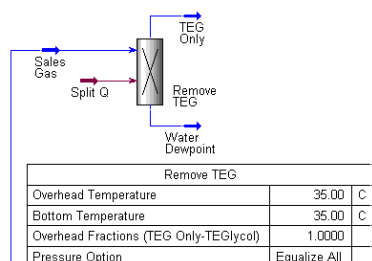
The next step is to add a Water Dew Point Property Correlation to the Water Dew Point stream.

5. Double-click on the **Water Dew Point** stream.

6. Open the **Properties** page on the **Worksheet** tab. The property correlations displayed are controlled using the buttons at the bottom of the **Properties** page.

Figure 6
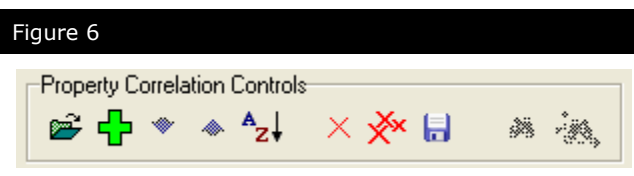
Append New
Correlation icon

7. Click the **Append New Correlation** button. The **Correlation Picker** view appears displaying all the available correlations in a tree format.

8. From the list of available correlations click on the '**+**' symbol to view additional sub-items for the **Gas** branch. Select the **Water Dew Point** correlation (see Figure 7) and click **Apply**. Close the **Correlation Picker**. The new correlation is added to the bottom of the list.
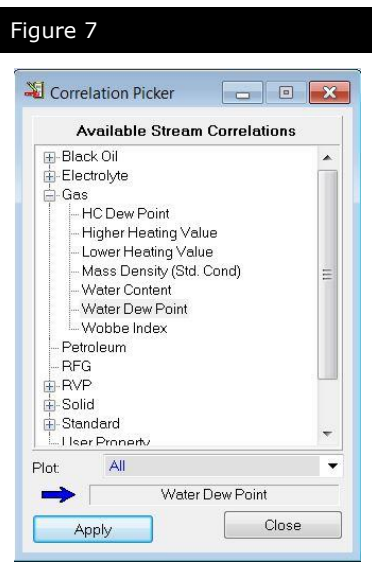
Figure 7

9. Locate the **Water Dew Point [Gas]** property correlation that was just added.

Figure 8
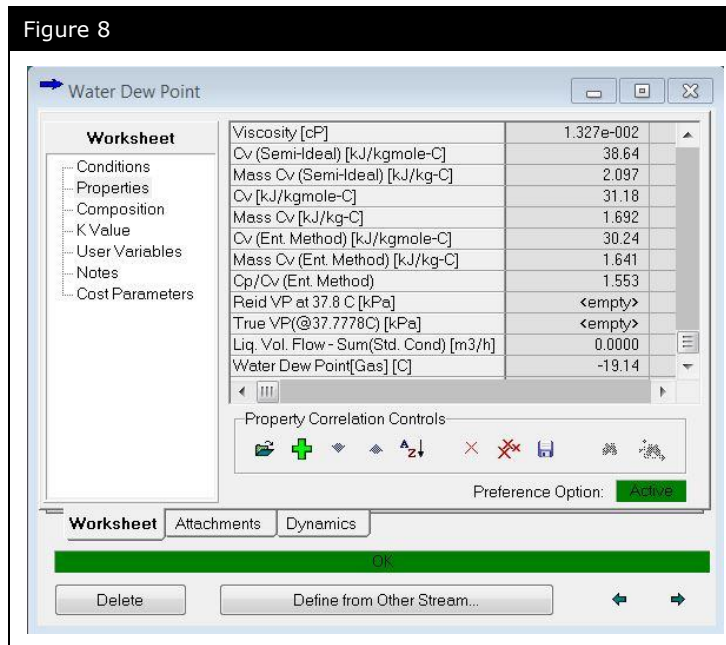
What is the water dew point temperature of the Sales Gas stream? Does it meet the required spec: -10°C (-14°F) at 6155 kPa (893 psia)?

_____

Exploring the Simulation

Exercise 1: Stripping Gas

The addition of stripping gas (a slip stream from Sales Gas) will enhance the ability of the Regenerator to remove water from the rich TEG. Take note of the current concentration of TEG in the Regen Bttms stream.

1. Add a Tee operation to split the Sales Gas into two streams. The strip gas stream is specified as follows:

    -   Flow = 50 kgmole/h (110 lbmole/hr)

The stream pressure is 6155 kPa which is too high for the Regenerator.

2. Add a heater to prepare the Strip Gas stream to be a feed to the Regenerator. Specify the following parameters for the heater:

    -   Product stream name = SG to Regen
    -   Product stream temperature = 70°C (160°F)
    -   Product stream pressure = 110 kPa (15 psia)

3. Connect stream SG to Regen as a feed to the Regenerator Reboiler.

Does the TEG concentration in Regen Bttms increase?

_____

Note: the sales gas now exceeds the dew point specification easily.

---

9. Reporting in UniSim Design

Introduction

Once you have finished a simulation, or during analysis, you may wish to obtain reports of the data that you have input and that UniSim Design has generated. Reporting data in UniSim Design can be achieved in a number of ways, such as:

- Report manager
- Print to File option
- Copy-Paste with Labels option
- Workbook and PFD customization
- Excel utilities

Learning Objectives

Once you have finished this module, you will be able to customize reports in UniSim Design using the Report Manager, customize the PFD and the workbook to display selected data and install and run an Excel utility to view data from the workbook.

Prerequisites

- Familiarity with the UniSim Design interface
- Ability to modify the workbook in UniSim Design
- Knowledge of Microsoft Excel

Report Manager

The Report Manager in UniSim Design allows the user to include data from all unit operations and streams in a UniSim Design case in any order. This information can then be printed. The information available through the Report Manager is the same information available if one prints a unit operation or stream report directly from the UniSim Design case.

Exercise 1

1. Open the solution case from the Gas Dehydration with TEG module, **4526.08.NGDehydrationTEG.usc**.
2. Go to the **Tools** menu, and select **Reports**. You are now in the Report Manager.
3. Click the **Create** button to create a new report. You are presented with a new window that allows you to customize the content of the report.

Information about operations and streams in UniSim Design used for printing is contained in objects called Datasheets.

4. Click the **Insert Datasheet** button to obtain a menu of all the information available in the case that can be included in the report:

Figure 1
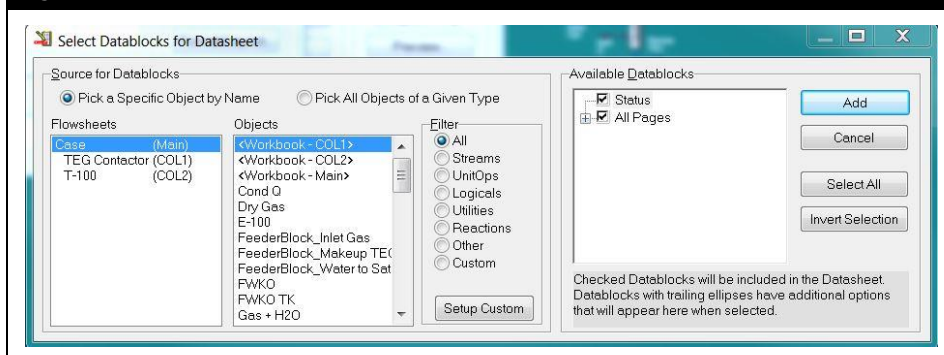
5. You can filter the lists by object type or by name, using the radio buttons at the top of the window. In this case, leave the radio button on **Pick a Specific Object by Name**.
6. Leave the **Flowsheets** selection at **Case (Main)** and choose stream **Sales Gas** under the **Objects** list. You will notice that all the datablocks available for stream Sales Gas have been selected by default in the **Available Datablocks** window:

Figure 2
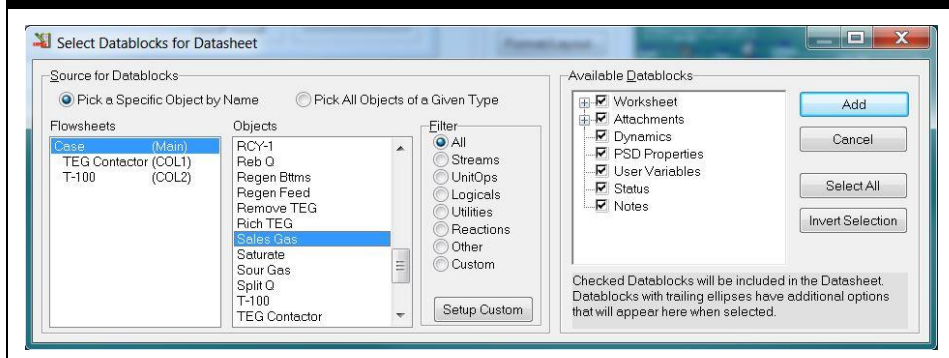
7. The only information we want to include in our datasheet is the stream conditions, so you need to click on the **+** next to the **Worksheet** option and deselect all the remaining selections (e.g. **Properties**, **Composition** and **K values**). You will also need to deselect **Attachments**, **Dynamics**, **PSD Properties**, **User Variables**, **Status** and **Notes**:

Figure 3
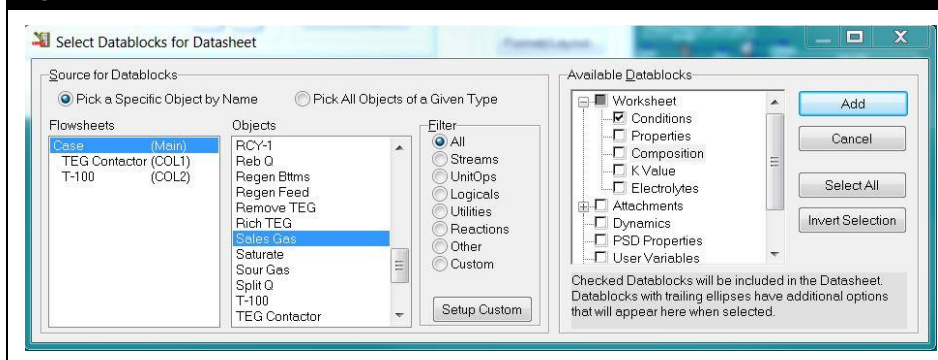
8. Click the **Add** button to add the **Conditions** for stream **Sour Gas** to the report. You will notice that the report now contains the conditions for stream Sales Gas.

9. Now, add the **TEG Regenerator** column **Design** Datablock to the report in the same way. (HINT: the **Flowsheets** selection must be left at **Case(Main)** in order to select the Design Datablock for a column.)

10. In the report manager, you can add information from the workbook as well as from streams and Unit operations. Add the **Unit Ops** page from <Workbook – Main> to the report.

11. We are now finished adding datasheets to the report. Close the **Select Datablocks for Datasheet** window.

12. On the **Report Manager** window, you can see that you can change the order in which the datasheets are presented in the report, and you can edit the content as well. In addition, you can change the name of the report. Change the name of this report to **Dehy Report**.

Figure 4
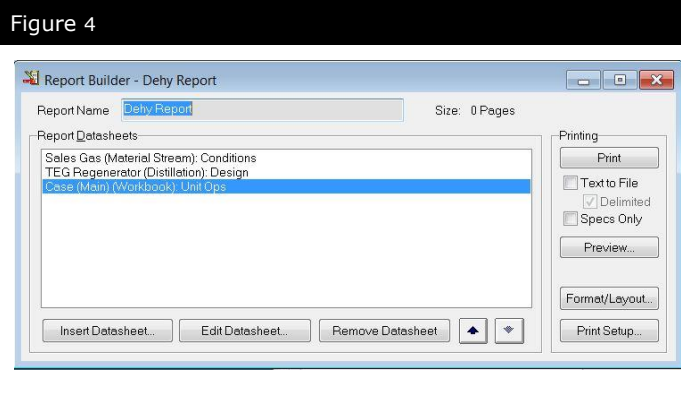
13. You can also change the format and layout of the report, as well as the unit set used in the report. Click on the **Format/Layout** button and select the **Field** Unit Set. This unit set will now always be associated with this report. Close the window.

14. You are now ready to **Print** or **Preview** the report. In this case, we will not print the report to paper, but we will preview it. Click the **Preview** button to see what the report would look like when printed.

Note that user specified values are identified on the printout with an asterisk, '*' ,next to them.

Save your case!

Customizing the Workbook

This topic was briefly covered in Modules 1 and 2. Additional detail will be provided here.

While the report manager is a useful interface for generating reports, it is not necessarily the most convenient method for transferring results from UniSim Design to Microsoft Excel or other tools, or even for printing the results directly from UniSim Design.

It is often easier to customize the workbook to generate the data set that is desired and then use the copy-paste functionality in UniSim Design to transfer the data to Excel for further editing or printing from Excel.

In addition to the normal copy-paste functionality, UniSim Design also allows the user to copy the data to the clipboard and include the data labels as well. This greatly reduces the formatting that is required to produce useful datasheets in Excel. This option is accessed by selecting **Copy with Labels** on the **Edit** menu, or by using the hot-key combination **CTRL+SHIFT+C**.

Additional Workbook Customization

In modules 1 & 2, you learnt how to add an additional workbook tab with customized properties. In this module, we will look at some additional options.

Sorting the Streams

The default behavior in UniSim Design is for the workbook to be sorted in the order that the objects were created. For example, the first stream that was added to the PFD will be the first stream in the workbook and the last stream created will be the last stream in the workbook. There may be times when you would prefer an alternate arrangement. This is easily accomplished with UniSim

Design. With the workbook open, simply open with **Workbook** menu and select **Order/Hide/Reveal Objects**. Alternatively, you can right-click on any object in the workbook and choose the **Order/Hide/Reveal** option in the list that appears.

By clicking on the **Ascending** or **Descending** radio buttons in the **Sorting** group box, you can direct UniSim Design to automatically sort the objects alphabetically in ascending or descending order. If you want to manually sort the objects to a particular order, simply choose the **Manual** option.

The **Order/Hide/Reveal** window also allows you to hide streams or operations that you are not interested in seeing. Simply select the stream that you want hidden and press the **Hide--->** button, the stream will move over to the **Hidden** column and will no longer appear on the active tab of the workbook. For example, if you hide the FWKO stream from the Material Streams workbook, it will still be displayed on the other tabs (e.g. Composition).

Exercise 2

Continue to use the TEG Dehydration case used in Exercise 1.

1. Open the workbook and create a new **Material Streams** tab following the procedure outlined in module 2.

2. Change the name of the new tab to **Feeds&Products**. Change the properties that are displayed to include: Temperature, Pressure, Mass Flow, and the Component Mass Flows for all the components.

3. Use the **Order/Hide/Reveal Objects** view to hide all streams except for the feed and product streams. The following streams should be visible: Gas to Contactor, Sales Gas, Sour Gas, Makeup TEG.

4. Use this workbook to ensure that the inflow of TEG (Makeup TEG) and the outflow of TEG (Sales Gas and Sour Gas) are equal.

5. Use the **Copy With Labels** option in UniSim Design to copy this workbook tab to an Excel worksheet.

6. Add the **Feeds&Products** workbook tab to the PFD as a workbook table.

Another useful feature of the workbook is the ability to reorganize the data in an inverted format. In this format, the property names are listed along the top of the workbook and the object information is listed in rows instead of in columns. To view this format, simply un-check the **Horizontal Matrix** checkbox in the lower left hand corner of the workbook.

This alternate view is an easy way to view the data and also provides another way of transferring the data to or from Excel.

Adding Process Information to the PFD

There are several ways to include process information with the PFD. One way, as was demonstrated in the previous exercise, is to add workbook tables to the PFD. You can also add stream tables to the PFD to display information on specific streams.

Some other methods include:
SHIFT+P, SHIFT+T, SHIFT+N, SHIFT+M, SHIFT+F, SHIFT+R hot-keys to display pressure, temperature, name, mass flow, mole flow, and description, respectively.

By using a custom colour scheme you can highlight streams with certain characteristics. For example, you can set up a colour scheme to show all streams below 50 ^{o}C in the normal colour, streams above 50 ^{o}C, but below 100 ^{o}C, in a cautionary colour (maybe yellow) and streams above 100 ^{o}C in a warning colour (maybe red).

A full list of all hot-keys is available by choosing the **Hot-key list** option on the **Help** menu.

Exercise 3 - Adding a Custom Colour Scheme

Colour Scheme Icon

1. Open the PFD view in the current case, if it is not already the active view.
2. Click on the **Colour Scheme** icon in the upper right-hand corner of the PFD window.
3. On the **PFD Colour Schemes** window that appears, click on the **Add a Scheme** button.
4. The default variable is **Temperature** and we will use this default in this exercise. Notice that there are several other choices that we could also have used.
5. There are five colours that can be used. You can adjust the cut points to create a colour scheme that will provide you with the behavior that you desire. For this example, the lower three cut points will not be changed. Only change the top cut point and make it the same as the third cut point (100 ^{o}C or 212 ^{o}F). This effectively reduces the colour scheme to a four colour system, but this is fine for this case.

Once this coluor scheme is active, you should see that the hottest streams on the PFD are shown in red and the cooler streams have other colours. The red streams should be: Regen Bttms, Regen Feed, Sour Gas, Lean From L/R, TEG to Pump, Pump Out.

It is obvious when the PFD is drawn with this scheme that we are pumping a very hot stream. This may not be recommended as it may require special insulation, materials, or seals in the pump. The process may be improved if the pump were moved to a position after the E-100 exchanger where the TEG stream is much cooler. This change could reduce the capital cost of the pump and potentially reduce the maintenance costs as well.

Creating Multiple PFD's

In UniSim Design, you have the capability of creating multiple PFD's for a single case. This can be a useful feature for very large cases, or for smaller cases when combined with additional colour schemes.

To create an additional PFD, open the **PFD** menu from the menu bar, and select **Add a PFD**.

This will create an additional PFD. With the additional PFD, you can return it to the default colour scheme, or change the stream label, or the positioning of the operations. You can also hide streams and/or operations on the second PFD to focus on a specific area of the flowsheet. Note, however, that if you delete streams or operations on either PFD, they will be deleted from the model. Streams or operations can be hidden on separate PFD's, but they should not be deleted.

It is important to note that both the original PFD and the second PFD are linked to the real time data. Anytime that the data is changed, this change will be reflected immediately on both PFDs.

Copying the PFD

Now that we have examined the process for adding process information to the PFD and changing the colour scheme on the PFD, we should examine the process for copying the PFD from UniSim Design into other applications like Microsoft Excel™ or Word™.

This is a very simple process. With the PFD open in UniSim Design, simply right-click on the background area. This will bring up the 'object inspection' window for the PFD. One of the options in this menu is **Copy Pane to Clipboard**. Select this option and a second window will appear; here you can choose the scaling factor. This affects the size of the bitmap file that is copied to the clipboard. Since it is possible to scale the graphic after it is imported into the other application, it is not too critical which scaling factor that you choose.

Once the pane is copied to the clipboard, go to the other application (Word, Excel, Powerpoint, etc.) and paste (**CTRL+V**) the clipboard image into that application.

> **The user should be aware that this process creates a static 'snapshot' of the PFD. Once the image is copied, it is no longer linked to the live data and any changes made to the UniSim Design case will not be reflected on the copied image.**

Exercise 4

1. Follow the steps described above to create a second PFD in the current case.
2. For the second PFD, select the default colour scheme and hide all of the operations except for the two exchangers.
3. Now hide all of the streams expect for the 8 streams directly connected to the two heat exchangers.
4. Change the stream label to show the stream's temperature instead of the stream's name.
5. Change the name of the second PFD to **HX Summary**.
6. Finally, use the **Copy Pane to Clipboard** functionality to transfer a snapshot of the modified PFD into Microsoft Excel.

Finding objects within the model

Another useful tool for viewing data in UniSim Design is the Simulation Navigator. This tool gathers all of the stream and operation object property views into a common location.

Simulation Navigator
Icon

To open the Simulation Navigator, either click on the **Simulation Navigator** icon in the tool bar, or select **Simulation Navigator** under the **Flowsheet** menu in UniSim Design.

Once the **Simulation Navigator** is open, you can see that all of the operations and streams are grouped according to their respective types. This allows you to quickly find streams if you know the name of the stream. Likewise, it allows you to quickly find the number of separators or columns in a model. Note that all of the streams are listed here, including those that are not part of the main flowsheet.

Now, the Simulation Navigator allows you to quickly view the properties for a stream, if you know the stream's name. But, how can you quickly find an object (stream or operation) on the PFD if you only know the object's name? The Simulation Navigator and the Workbook have a tool that is very useful for this exact task.

Once you have found the object with either the Simulation Navigator or the Workbook, you can locate it on the PFD as follows:

- From the Simulation Navigator, click the Find button located above the object tree (Figure 5)

- From the Workbook right-click on the stream name and select **Find in PFD**.

Figure 5
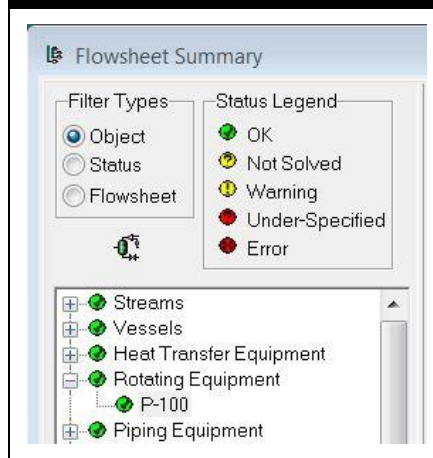
UniSim Design will open the PFD, and zoom into the PFD so that the selected stream or operation is in the centre of the view and the attached objects are also visible. This allows the user to zoom out to see a larger area on the PFD, while keeping the selected object in the centre of the view.

Alternatively if you have the PFD of a flowsheet open and you know that somewhere on that PFD there is a stream or flowsheet you want to locate you can right click on the PFD background and choose **Select Objects**. Find the object you require on the **Select Objects** window that appears. Press OK and note that now the object you choose is selected and flashing. If you cannot see the selected object press the **HOME** key on the keyboard to zoom the PFD on that object.

Excel Tools for Reporting

UniSim Design has a full OLE Automation interface. This feature has been used to create a number of tools to allow interface between UniSim Design and Excel. This module will focus on using the Workbook dump macro.

1. Open the workbook in the UniSim Design case. Customize the **Material Streams** tab to add the Component Mole Fraction of Water and the Mass Density to each stream. Ensure that the **Material Streams** page is the active page on the workbook.

2. Locate the file **UniSim Design WorkbookDump 1.0.1.xls** from your Starter disk and copy it to the hard drive of your machine. Any convenient folder is fine.

3. Double click on the Excel Spreadsheet to open it. Make sure macros are enabled in Excel.

4. You will see that all the workbooks available in the currently open case are listed in the window on the Excel spreadsheet. If they are not, click the **Refresh Flowsheet List** button.

5. Select the workbook for Case(Main) by clicking once on it, so it is highlighted in blue.

6. Click the **Dump Workbook** button. You will see the **Material Streams** page of the workbook being recreated in Excel. The user input values are shown in blue, in addition to having an asterisk next to them.

7. Now, switch to UniSim Design and make the **Compositions** page of the Workbook the active page. Return to Excel and click the **Dump Workbook** button again. Now, the **Compositions** page is shown in Excel.

Additional Excel Tools

Honeywell has other useful Excel tools:

- UniSim Design Stream Reporter (USD-SR) allows material stream conditions, properties and compositions to be easily reported onto a spreadsheet to easily create a Heat and Material Balance table, it also enables streams in different cases to be conveniently compared.

    UniSim Design Stream Reporter can be downloaded from the UniSim Design Customer Support Centre at http://unisim.supportportal.com.

- UniSim Design Browser can be used to set up OLE Automation links between UniSim Design and Excel without the user needing to write any Automation code. The Browser works by a series of custom Excel functions that interact with UniSim Design, and a graphical front end to simplify the writing of these functions. The functions can be copied, pasted and manipulated as required without any knowledge of VB programming.

- UniSim Design Excel Interface Tool (USE-IT) can be used to create and run case studies with UniSim Design with the input and output data stored in Excel.

    Since version R440 UniSim Design Browser has been integrated into the USE-IT tool. This can be installed from

    The Honeywell UniSim Design Suite installation files by using the 'Optional UniSim Components' option on the setup menu.

Answers to Questions

Chapter 1 – Getting Started

Page	Question	Answer
12	Normal Boiling Point of C7+, C7 and C8 respectively	110°C, 98.43°C, 125.7°C
	Ideal Liquid Density of C7+, C7 and C8 respectively	745.4 kg/m3, 686.8 kg/m3, 705.4 kg/m3
	Molecular Weight of C7+, C7 and C8 respectively	111.0, 100.2, 114.2
22	Vapour Fraction of GasWell 2 @ 7500 kPa and 10°C	0.9872
	Dew Point Temperature of GasWell 2 @ 7500 kPa	11.52°C
	Bubble Point Temperature of GasWell 2 @ 7500 kPa	-34.29°C
25	Critical Temperature and Pressure for GasWell 2 respectively	-11.98°C, 8984 kPa
36	**Using the Envelope Utility:**	
	Critical Point for GasWell 1	-1.079°C, 1.444e+004 kPa (Read in the Utility Design and/or Performance tabs)
	Cricondenbar (max pressure) for GasWell 1	1.630e+004 kPa (Read in the Utility Design and/or Performance tabs)
	Bubble Point Temperature for GasWell 3 @ 6000 kPa	Approximately -48°C (Read in the Utility Design and/or Performance tabs)
	Dew Point Temperature for GasWell 1 @ 4000 kPa	Approximately 98° (Read in the Utility Design and/or Performance tabs)
	GasWell 1 Temperature for 50% Quality @ 8000 kPa	Approximately -32°C (Read in the Utility Design and/or Performance tabs)
	Hydrate Formation Temperature for GasWell 2 @ 7500 kPa	Approximately 23°C (Read in the Utility Design and/or Performance tabs)
36	**Using the Workbook:**	(i.e. do an exact flash in the appropriate stream)
	Bubble Point Temperature for GasWell 3 @ 6000 kPa	-48.03°C
	Dew Point Temperature for GasWell 1 @ 4000 kPa	98.15°C
	GasWell 1 Temperature for 50% Quality @ 8000 kPa	-32.2°C
37	**Using the Hydrate Formation Utility:**	
	Hydrate Formation Temperature for GasWell 1 @ 5000 kPa	21.1195°C
	Hydrate Formation Temperature for GasWell 1 @ 7500 kPa	23.0220°C

Page	Question	Answer
	Hydrate Formation Temperature for GasWell 2 @ 5000 kPa	20.6794°C
	Hydrate Formation Temperature for GasWell 2 @ 7500 kPa	22.6077°C
38	Challenge: Dew and Bubble Point calculations on GasWell 3, at varying pressures, using the Property Table Utility	- Add the Property Table Utility for GasWell 3 - Variable 1 = Vapour Fraction, State (0, 1) - Variable 2 = Pressure, Incremental (100 – 10000 kPa) - Add Temperature as a Dep Prop - Calculate - On the Performance tab, view the table/plot for the points

Chapter 2 – Propane Refrigeration Loop

Page	Question	Answer
6	Pressure of Stream 1	1720 kPa
10	Molar Flow Rate of Propane	107.9 kgmole/h
	Pressure Drop across J-T valve	1469.20 kPa
	Temperature of the valve outlet (Stream 2)	-19.21°C
13	Compressor Energy in hp	218.521 hp
29	Chiller Duty (compressor running at 90% of max 250 hp and 72% efficiency)	Note: first remove the given/calculated Chiller Duty 9.885 e+005 kJ/h
29	Best Chiller Outlet Temperature achievable while still running the Compressor at a reasonable operating point (maintaining a chiller duty of 1.5 MMBtu/hr)	This cannot be calculated directly. Since if the chiller outlet temperature is removed and the duty reentered the simulation does not solve. This shows that UniSim Design cannot solve with every combination of variables, even though the degrees of freedom of the problem is zero. One way to do this is delete the compressor efficiency and specify the chiller duty. Now specify a chiller outlet temperature and manually iterate on this until the calculated efficiency is "reasonable". With this approach, a temperature of -5 °C gives an efficiency of 78.337%. Alternatively specify the efficiency and the chiller outlet temperature (hence calculate a chiller duty) and then use an Adjust operation to vary the chiller outlet temperature (the Adjusted Variable) until the chiller duty (the Target Variable) is 1.5 MMBtu/hr. This gives a chiller outlet temperature of -1.967 °C with a 72% efficiency.
30	What effect, if any, does a 95/5 mole % propane/ethane blend have on the refrigeration loop?	This blend is not as good a refrigerant and therefore less efficient. This means to achieve the same chiller duty requires a greater refrigerant flow rate and hence higher Compressor and Condenser Duties.
30	**Base Case:**	Flow = 107.9 kgmole/h

Page	Question	Answer
		Condenser Q = 1.587e+006 kJ/h
		Compressor Q = 218.5 hp
	New Case (5% C2, 95% C3):	Flow = 111.0 kgmole/h
		Condenser Q = 1.62e+006 kJ/h
		Compressor Q = 230.9 hp
31	Challenge: After creating a two stage refrigeration loop by adding an Economizer, what is the net compression in hp?	Stage1 comp duty = 65.63 hp Stage2 comp duty = 112.33 hp Net Compression = 65.63 hp + 112.33 hp = 177.96 hp

Chapter 3 – Refrigerated Gas Plant

Page	Question	Answer
10	Flow rate of Gas to Chiller	1440 kgmole/h
11	What information is required for the LTS separator to solve?	Gas to LTS Temperature (the LTS Feed Temperature)
12	Pressure of Sales Gas	6125 kPa
	Temperature of Sales Gas	10°C
15	Dew Point Temperature	-19.8°C
	Required dew point is -15°C, is the current dew point higher or lower?	Current dew point (-19.8°C) is lower than the required value of -15°C
	Assume pressure is fixed, what other parameter affects dew point?	Mole Fraction (composition) also affects dew point.
	How can we change the dew point in the simulation?	Since dew point pressure is fixed in the simulation, the dew point temperature can be modified by changing the Chiller outlet (Gas to LTS) temperature. A change in Chiller outlet temperature will change the composition (phase fraction) of the Gas to LTS stream (it is a two phase stream going to the separator).
19	What is the Chiller Outlet Temperature to achieve the Dew Point specification?	-15.18°C
22	Flow rate of propane in the Refrigeration Loop	156.9 kgmole/h Right click on sub-flowsheet icon and choose **Open** PFD to view the Refrigeration Loop PFD.
23	Available UA for the Gas-Gas Exchanger is only 2e+005 kJ/°C·h. Making the necessary modifications to the exchanger design to achieve this UA; how do these modifications	De-activate the Temp Approach spec and activate the UA spec. Go to the Details page of the Performance tab to view the temperature approach (Min. Approach) and LMTD, which have increased. Min Approach = 7.301°C (up from 5°C)

Page	Question	Answer
	affect the LMTD and Temperature Approach?	LMTD = 9.151°C (up from 7.131°C)
23	Challenge: Replace the single-sided cooler operation with the shell and tube exchanger that will actually be in the plant.	-Delete the chiller in the main PFD and in the sub-flowsheet -Add a shell and tube heat exchanger operation on the main PFD -Connect the streams from the main PFD to the shell side of the new heat exchanger, and specify a Delta P of 35 kPa -Connect the streams from the sub-flowsheet to the tube side (on Design\Connections page of heat exchanger by changing the tube side sub-flowsheet to the refrigeration loop) and specify a Delta P of 7 kPa
26	What First Stage Compressor Outlet Pressure (stream 4) will result in the minimum power usage in the Refrigeration Loop?	800 kPa is the First Stage Compressor Outlet Pressure (stream 4) which results in 176.02 hp usage (the minimum power usage in the Refrigeration Loop). This can be observed by clicking the Results button in the Case Studies Setup window and selecting either Table or Graph format.

Chapter 4 – NGL Fractionation Train

Page	Question	Answer
13	Mole frac of Methane in DC1 Ovhd	0.97
15	Flow rate of the overhead product, DC1 Ovhd.	1350 kgmole/h
16	Flow rate of C2 and C3 in DC2 Btm	C2=0.66; C3=106.1 kgmole/h
	Ratio of C2/C3	0.66/106.15 = 0.00626 You can also allow USD to calculate the ratio for you by adding a component ratio spec. To do so follow the instruction on page 16 (points 3, 4 and 5). Leave the component spec inactive for now but notice that the current value is calculated for you regardless.
17	Flow rate of DC2 Ovhd	307 kgmole/h
18	Mole Fraction of C3 in overhead and bottoms products	C3 in DC3 Dist = 0.9207 C3 in DC3 Btm = 0.2547
22	Challenge 1: UA of the De-Methanizer Reboiler? Create an internal stream in the column flowsheet that represents the liquid that flows from the bottom tray of the reboiler, which can then be added to a heat exchanger in the main flowsheet. Use steam to exchange heat with	UA is dependent on both sides of a heat exchanger. The column reboiler is similar to a heater + separator; can't get UA value from this configuration (can only get UA value from a proper heat exchanger). In column view (copy Reboiler tray 10): -Go to column runner, flowsheet tab, add internal stream -Select stage 10-main, type = liquid, check Export so that the stream will appear in the main flowsheet, Run In main view: -Add a heat exchanger with the following connections; tube

Page	Question	Answer
	the process.	side inlet=(internal stream added), tube side outlet=2, shell side inlet=1 (steam), shell side outlet=3, Delta P for shell side is 5 psi and tube side is 0
		Add a Set operation (live data): -Target = stream 2 (tube side outlet temperature) -Source = DC1 Btm
		UA of De-Methanizer Reboiler: -Open the heat exchanger view, Details page of the Performance tab
		UA* = 7.11e+04 kJ/C-h
		*If using Weighted Heat Exchanger Model, which is recommended since the steam is condensing
23	Challenge 2: Given additional geometry/size and operating data for valve VLV-100, use the P-F Relation specification instead of Delta P. Check that the valve stays within the pressure range for stream DC3 Feed when operating at steady state.	-Delete the pressure specification in stream DC3 Feed
		- In valve VLV-100:
		-On Rating tab, Sizing page, set the Valve Manufacturer to Universal Gas Sizing and characteristic to Linear
		- On the Design tab, Parameters page, select P-F Relation for Pressure Drop Parameters
		-Enter Valve Opening and Conductance
		Stream DC3 Feed Pressure = 1653 kPa
		The pressure for stream DC3 Feed is within the acceptable range when operating at steady state (1600 – 1800 kPa)

Chapter 5 –
Oil Characterization

Page	Question	Answer
14	The two lowest boiling points for the hypocomponents	NBP[0]94* @ 94°C NBP[0]186* @ 186°C
20	Why doesn't the calculated hypocomponent data match the curve data supplied in Figure 3?	The input assay data (Figure 3) does not include Light Ends, while the calculated data includes both hypocomponents and Light Ends.
21	Are the results from the BP Curves Utility a good match for the input assay data? Why?	No, for the same reason.
22	Challenge: Calculated temperatures at the 50% and 75% cut points	50% Cut Point, TBP = 285.9°C 75% Cut Point, TBP = 387.2°C
	How do the results of the BP Curves utility without Light Ends compare to the input assay data?	Splitting the Light Ends from the hypocomponents using the Component Splitter allows for a like for like comparison of the calculated hypocomponent data versus the input assay data. The results of the BP Curves utility without Light Ends are a good match to the input data. For example, at 50% the temperature input was 287°C versus the calculated TBP of 285.9°C (very close).

Chapter 6 – Two-Stage Compression

Page	Question	Answer
11	Can the values in streams LD1 Out and LD2 Out be used as the guess for the Recycle outlet?	Since both LetDown valve outlets (also the recycle inlets) are known, these streams (LD1 Out and LD2 Out) are good starting points for the Assumed stream (the guess for the Recycle).
11	**Valve Parameter Comparison:**	
	LD1 Out (Temp, Press, Flow)	42.41°C (calc), 1725 kPa, 17.51 kgmole/h (calc)
	LD2 Out (Temp, Press, Flow)	38.75°C (calc), 3450 kPa, 224.2 kgmole/h (calc)
	Is Composition known for LD1 Out?	Yes
	Is Composition known for LD2 Out?	Yes
15	How many iterations did each Recycle need to converge?	1 iterations (RCY-1), 2 iterations (RCY-2) (Sort by Iteration on Tables page of Monitor tab – note the number of iterations will depend on the starting values, which will depend on the precise steps and values used to build the simulation. However, both recycles should converge with very few iterations).
	How close are the Inlet and Outlet stream variables for each Recycle?	Identical or almost identical
	Are the Vapour Fractions identical for the Inlet and Outlet?	The Vapour Fractions are almost identical for RCY-1 and RCY-2 (see Recycle Stream Comparison below)
15	**Recycle Stream Comparison:**	
	RCY-1	Inlet Vf = 0.1527 Outlet Vf = 0.1527
	RCY-2	Inlet Vf = 0.2950 Outlet Vf = 0.2949
29	Are there any unit operations with balance errors? Which ones?	The Simulation Balance Tool trace window reports "Mass NOT Balanced". Open the Simulation Balance Tool and notice the message: "Run with Operations Exceeding Tolerances". Go to the Summary tab for a list of unit operations with balance errors. The recycle unit operations have the following balance errors. RCY-1: absolute and relative mass errors relative mole errors absolute and relative energy errors absolute component errors (n-Hexane) RCY-2: relative mole errors absolute energy errors
	Why do you think these unit operations have balance errors?	These recycles use an iterative numerical method to achieve convergence therefore the solution accuracy depends on the tolerances specified and the initial

Page	Question	Answer
		estimates.
	Can you think of a way to reduce the errors?	Tightening tolerances. Modify the appropriate sensitivity of the Recycle operations on the Adjust/Recycle tab of the Simulation Balance Tool.
29	Did reducing the sensitivity resolve the balance errors?	Yes. Overall Mass Balance Monitor shows "Mass Balanced" status indicating that the overall mass balance is satisfied to within the tolerances specified by the user + SBT should show no operations exceeding tolerances
	How did it achieve this?	This was achieved by tightening the tolerances so that the recycles are converging to a higher accuracy.
35	Outlet pressure of Pipe-100	5900 kPa
44	Exercise 5: After adding a Compressor Curve for the Stage 2 Compressor, will the existing Compressor be able to achieve the outlet pressure desired (6900 kPa)? Will the addition of a third stage of compression be required?	First delete the specified adiabatic efficiency and Stage 2 Out pressure. -Open the Stage 2 Compressor view and go to the Curves page on the Rating tab -Click the Add Curve button and enter the Speed, Flow, Head and Polytropic Efficiency data provided in Exercise 5 -Close the window -Select Polytropic Efficiency -Check "Activate" for the added curve and also -Check "Enable Curves for SS" -Click the Plot Curves button to view the operating point within the curve Stage 2 Out pressure = 6595 kPa The existing compressor was not able to achieve the desired outlet pressure of 6900 kPa and the addition of a third stage of compression is required. Perhaps with a faster compressor speed the desired outlet pressure could be achieved, however we do not have other compressor curves to run.
44	Challenge: Can you reduce your convergence time by eliminating one of the recycle unit operations?	Looks like your boss is right! Only one recycle block is needed in this flowsheet, at the inlet to the IS Sep. Having a single recycle block at the inlet to the IS Sep allows for both recycle streams to be converged. The Recycle Assistant also advises this recycle location and the deletion of the old ones.

Chapter 7 – Acid Gas Sweetening w/ DEA

Page	Question	Answer
9	Flow rate of water in stream FWKO	14.32 kgmole/h
11	Concentration of H2S and CO2 in the Sweet Gas stream	H2S = 0.0000 CO2 = 0.001583 Note that for gas streams "concentration" almost always refers to mole fraction.

Page	Question	Answer
15	Flow rate of stream Makeup H2O	0.7065 kgmole/h
		(After closing the recycle loop this becomes 5.453 kgmole/h)
20	CO2 vol% in the Sweet Gas	0.1708 vol%
		Note that for gas streams vol% does not refer to liquid vol%. For gas streams volume fraction = mole fraction, and thereby to calculate vol% multiply mole frac by 100.
		CO2 (mole frac) = 0.001708 CO2 (vol%) = 0.001708*100 = 0.1708
	H2S vol ppm level in the Sweet Gas	0.2391 vol ppm
		Recall that volume fraction = mole fraction for gas streams. The vol ppm of H2S can be calculated by either:
		1. Multiplying the mole fraction of H2S by 1e6 using a spreadsheet, OR
		2. Changing the basis to mole flow which will display more significant figures, then calculate: (H2S mole flow/Total mole flow)*1e6
	Have the following pipeline specifications been met? Less then 2 vol% CO2 Less than 4 ppm (volume) H2S	Yes, the pipeline specifications have been met: **CO2:** 0.1708 vol% **<** 2 vol% **H2S:** 0.2391 ppm (volume) **<** 4 ppm (volume)
23	Exercise 1: What changes are necessary in the simulation to double the flow rate of gas to the plant?	More gas to the plant requires more amine. -Double the flow rate of the Sour Gas (feed) stream -Double the amines recirculation rate (Std Ideal Liq Flow) in streams DEA to Cool and DEA to Contactor -Double the Regenerator Reboiler Duty specification on the Monitor page of the Design tab, since more amines require more energy to regenerate. This is a very simple approach and likely could be optimized.

Chapter 8 – Natural Gas Dehydration w/ TEG

Page	Question	Answer
8	What is the Vapour Fraction of Stream Gas+H2O? (it should be less than 1.0 to ensure saturation)	0.9999
9	How much water is removed by the Separator?	1.131 kg/h total stream flow Read from the FWKO stream out of which 1.13074 kg/h H2O component mass flow
12	Flow Rate of Stream Makeup TEG	-6.5234e-003kgmole/h (After closing the recycle loop this becomes 4.7041e-004 kgmole/h)
16	Hydrate Temperature of the Sales Gas stream	1.2385°C Copy the stream, switch to Peng Robinson fluid package and add a Hydrate Formation Utility to the stream
	How does the Hydrate Temperature of the Sales Gas stream compare with the Hydrate Temperature of the Gas to Contactor stream?	Gas to Contactor stream Hydrate Temperature = 18.14°C Sales Gas stream Hydrate Temperature = 1.2385°C The Sales Gas stream Hydrate Temperature is much lower than that for the Gas to Contactor stream. Hydrate will not form until a lower temperature for the Sales gas stream since the water in this stream has been removed by the TEG Contactor operation. The higher the amount of water in a stream, the greater the probability that hydrate will form near normal operating temperatures. By removing the water (with TEGlycol for example) the temperature at which hydrate forms is lowered, potentially out of operating temperature range, and averting problems in the pipes.
19	What is the water dew point temperature of the Sales Gas stream? Does it meet the required spec: -10°C (-14°F) at 6155 kPa (900 psia)?	Sales Gas stream: water dew point temperature = -19.14°C pressure = 6155 kPa The Sales Gas stream meets and exceeds the required spec.
20	Exercise 1: SG to Regen enters as a feed to the Regenerator Reboiler. Does the TEG concentration in Regen Bttms increase?	Yes, the TEG concentration increases in the Regen Bttms; from 0.9115 to 0.9991 Less water in the Sales Gas stream results in improved TEG recovery in the Regen Bttms stream.