# **3** Chemicals Tutorial

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#### 3-2 Chemicals

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

# 3.1 Introduction

In this tutorial, a flowsheet for the production of propylene glycol is presented. Propylene oxide is combined with water to produce propylene glycol in a continuously-stirred-tank reactor (CSTR). The reactor outlet stream is then fed to a distillation tower, where essentially all the glycol is recovered in the tower bottoms. A flowsheet for this process appears below.



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

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

The simulation will be built using these basic steps:

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

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

# 3.2 Steady State Simulation

# 3.2.1 Process Description

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



The propylene oxide and water feed streams are combined in a Mixer. The combined stream is fed to a Reactor, operating at atmospheric pressure, in which propylene glycol is produced. The Reactor product stream is fed to a distillation tower, where essentially all the glycol is recovered in the bottoms product.

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

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

# **3.2.2 Setting Your Session Preferences**

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

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

Simulation	Ganetal Options	P7 Han Grand Frankla			
<b>Options</b>	J Allow Multiple Stream Cornections	V Use input Expens			
Desktop	View New Steams upon cleanun	V Confirm Mode Switches			
Naming	Record Time When Notes Are Modified	Enable Single Click Action			
Tool Tips	F Enable Cross Hairs On PFD	Enable Cell Edit Button			
Dynamics Performance Licensing	Errors T Displey Errors in Trace Window Displey Numerical Errors in Trace Window (Ignore, Them in Dynamics Mode)				
RTI Server	Show Property Package Warning				
Column	I⊽ Show Property Package Warning				
Status Window	Eroperty Correlations	······································			
Trace Window	P Activate Standard Property Correlations				
	Confirm Before Adding if Active Correlations are Present				

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

### Creating a New Unit Set

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

1. In the Available Units Sets list, select Field.

The default unit for Liq. Vol. Flow is barrel/day; next you will change the Liq. Vol. Flow units to USGPM.

Variables	Available Unit Sets		
	Field		Clone
Comes			Deiete
	Unit Set Name Field	9/1 	BAY LISPES
	Display Units		
	Vapour Fraction	Unitiess	Yew.
	Temperature	F F	Add
	Flow	bmole/hr	Urriete
	Liq. Vol. Flow	barrel/day	
	Molar Density	bmole/it3	

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

The default Preference file is named **HYSYS.prf**. When you modify any of the preferences, you can save the changes in a new Preference file by clicking the **Save Preference Set** button. HYSYS prompts you to provide a name for the new Preference file, which you can later recall into any simulation case by clicking the **Load Preference Set** button. 6. From the list, select USGPM.

Variables	Available Unit Sets			
Unitz Formats	Field-USGPM Field-USGPM HoverTextUnitSet1 HoverTextUnitSet2 Unit Set Name	ield-USGPM	י ר ד ד ד	Clone Delete
	Display Units	2012 - January 1997 - Santan Barran and Santan S 2012 - Santan		
		Unit	<u> </u>	Yiew
	Pressure	psið ihmole /hu		Add
	Mass Flow	b/h	- <u></u>	متعلم 1
	Lig Vol Flow	barrel/day	<u> </u>	
Cinclation M	Linergy	cm3/s barel/day barel/hr USGPM USGPH T d ft3/hr		True come f

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

# 3.2.3 Defining the Fluid Package



New Case Icon

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

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

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

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

1. (	Click	the	New	Case	icon.
------	-------	-----	-----	------	-------

The Simulation Basis Manager appears. 2.

· · ·				and the state of t	dour multiple provide and	A
Component Liste		-1	1			
Master Component Las	¥1994					
	Add					
	Deinte					
	Сару	ļ				
	import.					
	Egool.	J				

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

# Creating a Fluid Package

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

Component List Selection	Property Package Selection (none) Antoine Pkg Antoine Astime Steam Braun K10 Chan Nut Esso Tabular Estended NRTL GEEDS General MRT	Property Package Filter C All Types C EOS: C Activity Models C Drao Seador Models C Vapour Press Models C Miscolaneous Types		
TIM I been 1969293000	Component List Selection		Advanced Thermodynami	



3-8

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

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

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

Package Filter
o Seader Models
our Press Models
stareous Types
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The Property Pkg indicator bar at the bottom of the view now indicates UNIQUAC is the current property package for this Fluid Package.



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



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

### **Selecting Components**

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

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



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

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

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

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

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



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

Add Component	12C30xide	Match Propyleneo	inu Fans
Traditional Electrolyte		© Sim Name C Full Name / Synorym	C Formula
Hypothetical Other	-Add Pure	BisPhenol p.p'-(sopropylidenebisphenol)	C19H1602
	(Subsidiater)	12-CIC3 Propylene Dichloride 12-C3diol Propylene Glycol	C3H6C12 C3H6O2
		C3-Calourate riopytalecationale	C4noU3
	<u>Yiew Component</u>		

The component now appears in the Selected Components List.

ilter	s statut	×)
Pro	perty Package Filter	
Г	Recommended Only	
[ <n< td=""><td>one&gt;</td><td></td></n<>	one>	
-Fan	nily Type Filter	
5	Use Filter	
Г	Hydrocarbons	
Г	Solids	
Г	Miscellaneous	
Г	Amines	
Г	Alcohols	
Г	Ketones	
Γ	Aldehydes	
<u> </u>	Esters	
Ľ	Laboxylic Acids	
-	Halogens	
-	Phenole	
'n	Ethers	
г	User-Defined	
	Al	
	Invert	

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

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

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

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

Add Component	Selected Components		Components Avail	able in the Component Library	an a
Components	12C30xide		Metch pro	pyle	View Filters
Electroixe			🐨 Sim Name	(* Full Name / Synonym	C Formula
Other		< Add Pure	TriC3=Glycol 12-C3diol	Propanol. ((1-Mathyl-1,2-Ethane Propylane_Glycol	delibistanelibis- C9H2 C3H8O2
		(-Substitute->			
		Remove>			
		Sort Liet		·	
		View Component			
			F Show Synamy	ns / Custer	

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

Finally, you will add the component H2O.

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



15. The final component list appears below.

#### **Viewing Component Properties**

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

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

Component Identifical	<b>6</b>
Component Name	12-0340
Family / Class	Alcohol
Chem Formula	C3H8O2
ID Number	500
Group Name	
CAS Number *	
CH3 CH2 CH (OH)2	
CH3 CH2 CH (OH)2 Usej ID Tags	mber Tao Tent I
0H3 CH2 CH (0H)2 User ID Tags Tag Nu 1 1 4	emply> Tag Text emply> Not Spec'd

A component can be removed from the Selected Components list by selecting it and clicking the **Remove** button or the **DELETE** key. The Component property view provides you with complete access to the pure component information for viewing only. You cannot modify any parameters for a library component, however, HYSYS allows you to clone a library component into a Hypothetical component, which can then be modified as desired. Refer to Chapter 3 - Hypotheticals in the Simulation Basis manual for more information on cloning library components.

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

### **Providing Binary Coefficients**

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

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

-Activity Model	nteraction Par	Arrielena		en an		بنين مير المراجع مرد ا	
Coeff Matrix To	View:	(° Ali	CBL		9.2 )		Coeff Estimation
house and		and a start of the second s		ىسى <del>ئۇرى</del> رىيى بىرىيە . شە		الشطوره	C UNICACILE
Disk Ostan	12C3Gxide	12-C3diol	H20		ं ा हा		C Immiscible
12C3Olide	*		-71,309				
12-C3diol			-335.032				Individual Par
H20	823.550	-5.027					Unknowns Date
							Contraction of the second second
The second second							ALL Brianes
51X 187						· • • • • • • • • • • • • • • •	Reset Parama
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Sec. W2 88879	terestation of the communities	<b>ا</b>	ا در را به معاند و از را بر ا	ا مىسىيە بىلا ئىرىلىلامىيە	] السنديدينيكيسيسيدالـغ		Land Street D

In the Activity Model Interaction Parameters group, the Aij interaction table appears by default. HYSYS automatically inserts the coefficients for any component pairs for which library data is available. You can change any of the values provided by HYSYS if you have data of your own. In this case, the only unknown coefficients in the table are for the 12C3Oxide/12-C3diol pair. You can enter these values if you have available data, however, for this example, you will use one of HYSYS' built-in estimation methods instead.

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

- 2. In the Coeff Estimation group, ensure the UNIFAC VLE radio button is selected.
- 3. Click the Unknowns Only button. HYSYS provides values for the unknown pair. The final Activity Model Interaction Parameters table for the Aij coefficients appears below.

Activity Model Ir	Neraction Para	Defeit	<u>Arian (Arian)</u> Arian (Arian)
Coalt Matrix To	View	° 🗛 👘 🗏	C Bi
	12C3Obide 1	12-C3dia	H20
12C30xide		170.570	-71.909
120261	787.060		-335.033
12		taken a second state of the second state of th	a de selementar en al a del sus popo popo popo de se de se

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

#### A Basis Icon

# 3.2.4 Defining the Reaction

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

-Rien Components	Reactions		Reaction Sets	
12C30xide 12-C3dio		Mew Rgn.	Global Rxn Set	Yiew Set
H20		Add Exn.		Add Set.
		Dekte finn		Dalete Set
		Copy Rxn	Assoc Fluid Picos	Copy Set
				Import Set .
	彩 開 经济防运			Export Set.
Add Comps.				Add to FP
Add Congs				Export Set . Add to FP

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

 $H_{\bullet}O + C_{\bullet}$ 

1. Create and define a Kinetic Reaction.

These steps will be followed in defining our reaction:

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

$$H_2O + C_3H_6O \rightarrow C_3H_8O_2 \tag{3.1}$$

### Selecting the Reaction Components

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

To add or remove a component, click the Add Comps button. The Component List View appears. Refer to the Selecting Components section in Section 3.2.3 - Defining the Fluid Package for more information. 3-17

### **Creating the Reaction**

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

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



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

S Kinetic Beach	on Ren 1		
Stoichiogetry and	Rate Info		
*Add Comp**	Mole WI. Stoich D	ceff Fwd Order R	ev Oider
Eplance	Balance Ellior Reaction Heat (25 C)	0.00000 <empty></empty>	
	Base Perameters	The Street Street	

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

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

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

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

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

Kinetic Heastin	on: Rxn-1	1		
Staichiogeby and	Rate Info			
Component	Mole Wt.	Stoich Coeff	Fwd Order	Rev Order
H20	18.015	•1.000	1.00	0.00
12C30xide	59.080	-1.000	1.00	0.00
12-C3diol	76.096	1,000	0.00	1.00
"Add Comp""				
			1. Siterar	and the state of the second
Bglance	Balance Error Reaction Hea	(125.C) -3.9e	0.00000 +04 Btu/Ibmole	
Stoichiomotry	Basis Para	meters		

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

HYSYS provides default values for the Forward Order and Reverse Order based on the reaction stoichiometry. The kinetic data for this Tutorial is based on an excess of water, so the kinetics are first order in Propylene Oxide only. 9. In the Fwd Order cell for H2O, change the value to 0 to reflect the excess of water. The Stoichiometry tab is now completely defined and appears as shown below.

et a state of the	an total	A CARLEY	and the second		
Concornert	Hole WD	Strich Coeff	Furt Order	Rev Order	1887
H20	18.015	-1.000	0.00	0.00	
12C3Oxide	58.090	-1.000	1.00	0.00	
12-C3diol *Add Comp**	76.096	1.000	0.00	1.00	
Balance	Balance Ettor Reaction Heat	(25 C) -3.9e+	0.00000 04 Btu/Ibmole		

The next task is to define the reaction basis.

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

Notice that the default values for the Forward Order and Reverse Order appear in red, indicating that they are suggested by HYSYS. When you enter the new value for H2O, it will be blue, indicating that you have specified it. You can have the same reaction occurring in different phases with different kinetics and have both calculated in the same **REACTOR**. 14. In the **Rxn Phase** cell, select CombinedLiquid from the drop-down list. The completed **Basis** tab appears below.



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

- 15. Click the **Parameters** tab. On this tab you provide the Arrhenius parameters for the kinetic reaction. In this case, there is no Reverse Reaction occurring, so you only need to supply the Forward Reaction parameters:
- 16. In the Forward Reaction A cell, enter 1.7e13.
- 17. In the Forward Reaction E cell (activation energy), enter 3.24e4 (Btu/ lbmole).

The status indicator at the bottom of the Kinetic Reaction property view changes from Not Ready to Ready, indicating that the reaction is completely defined. The final Parameters tab appears below.

Forwa	d Reaction	Equation Help			2
A	1.7000e+013	r = k*1(Basis) k	"f(Basis)	H. W.	
E	32400	$k = A^* \exp \{-E\}$	/8T)*T*8	1 8 · · ·	
134	entroy i	k' = A'*exp{-E	'/AT}*T*B	1	
Reyer	e Reaction	T in Kelvin			
<u>A'</u>	(empty)	J			
E	<empty:< th=""><th>1</th><th>· • ·</th><th></th><th></th></empty:<>	1	· • ·		
1n.	I cembrys		8	8	

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



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

### **Creating a Reaction Set**

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



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The same reaction(s) can be

in multiple Reaction Sets.

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

Reaction Set Set 1
Berne Set-1
Set Type Unknown Advarced
Active List DK Inactive List Dpendions Atlached      (empty>     (empty>
Aran Astron

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

Active List	OK
Rxn-1	12
<emply></emply>	

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

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

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

×	adde Tor is	50. M				1 ( ) ( ) ( ) ( ) ( ) ( ) ( ) ( ) ( ) (		
12C30xid	o i	Ran-1	Vie	• Fign. 1	Global Rim Set	<u> </u>	w Set	
12-C3diol H20			Ad	Ban.	36(-)		d Set.	
and the second	and the second		ar sis ≱∯el	eta Pixri		Da	inte Sei	
			Cop	vRxp	August Di 14 Dinas	<u></u> Ca	oy Set	1990 - 1882 - 1
		and the				ino	ort Set.	1120 1
						Exp	of Set.	18-
Add C	omgs					A	d to FP	
A State of the second s						det Mar		4

## Making the Reaction Set Available to the Fluid Package

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

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

igure ozo	
≫î Add 'Set-1'	
Basset NC 3 PP U	NGUAC Ideal

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



Current Fluid Pa	ckages		Flowsheet	- Fluid Pkg Assoc	iations	<u>a</u> tai
Basis-1 NC	3 PP UNIQUAC IN	K <u>Vievi</u>	I) / P	Case (Main)	Fluid Pkg To Use Basis-1	<u>1 - 1 - 1 - 1 - 1 - 1 - 1 - 1 - 1 - 1 -</u>
		<u>A</u> dd				
		Belete				
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	No. The No.	import	内国家			
		Summer of Street		S STUES		1
		C C C C C C C C C C C C C C C C C C C	Def	nut Fluid Pikg	Basis-1	

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

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

3-25



# 3.2.5 Entering the Simulation Environment

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

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

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

	= x= x>	👁 🐨 🛛 🌡	Enviro Enviro	ment Case Mode: Stead	(Main) v Stata
<ul> <li>Workbook - Case (Main)</li> </ul>				الداعاء	Case (Main)
Name **	lew **				1 <b>(2</b> )
Vapour Fraction Temperature (F)				[]	
Pressure (psia)		10.00 Hilling and \$1.00 H			
Mass Flow [b/hr]				·	661
Liquid Volume Flow [barrel/day] Heat Flow (Blu/hrl	·····				
(man a )					
Material Streams Compositions	Energy Steams	Unit Upe			x q P
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There are several things to note about the Main Simulation environment. In the upper right corner, the Environment has changed from Basis to Case (Main). A number of new items are now available on the Menu and Toolbar, and the Workbook and Object Palette are open on the Desktop. These two latter objects are described below.

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

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

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

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

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

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



ايد



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

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

# 3.2.6 Using the Workbook

### **Installing the Feed Streams**

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

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

lame	Prop Oxide	** New **	
Apout Fraction	<empty></empty>		
emperature [F]	<empty></empty>		
Sressure (psia)	<empty></empty>		
totar Flow [bmole/hr]	<empty></empty>		1
dass Flow (b/h)	<empty></empty>		
iquid Volume Flow [USGPM]	<empty></empty>		
leat Flow [Btu/hr]	<empty></empty>		
·	ALL POTTO CO	a. Linana	r <del>ina an</del>

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

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

4. Click in the Temperature cell for Prop Oxide.



Workbook Icon

HYSYS accepts blank spaces within a stream or operation name.

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

Hame	Prop Oxide	** New **	I
Vapour Fraction	(emply)	terrege and million and	
Temperature (F)	75.00	F 💌	
Pieseure (peia)	<empty></empty>		
Molar Flow (Ibmols/hr)	<emply></emply>	1	[
Mass Flow [b/hr]	<empty></empty>		[
Liquid Volume Flow [USGPM]	<empty></empty>		l I
Heat Flow (Btu/hr)	<emply></emply>	I	
·····			

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

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

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

Name	Prop Oxide	** New **	<u> </u>
Vapour Flaction	<empty></empty>		
Temperature (F)	75.00		j †
Pressure (psia)	1.100	atm 💌	
Molar Flow [Ibmole/hr]	<empty></empty>	atn 🔺	
Mass Flow (lb/h)	<empty></empty>	al	
Liquid Volume Flow [USGPM]	<empty></empty>	kg/cm2 🛄	
Heat Flow (Blu/hr)	<empty></empty>	psia 5(8)7	
		tor	
		mmHa(OC) 🚿	Puinter
Material Streams   Comp	ostions Energy	SUCCESSION OF SUCCESSION	

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

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

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

#### **Providing Compositional Input**

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

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

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

Input Composition	for Stream: Prop Ux	ide 🔀
2 TY 4 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	MoleFraction	Composition Basis
12C30xide	<empiv></empiv>	Mole Fractions
12-C3dio	(empty)	- C Mass Fractions
H2U	<empty></empty>	
		- TUT Trease Lighters
e and a second second		C Mole Flows
and the second		C Mass Flows
and the second	· ••••••••••••••••••••••••••••••••••••	C Datt - D
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1	201424444444444444444444444444444444444	Composition Council.
A MO AND AND A MARKED AND A MAR		Erase
an i a station and a statio		[
		Normalize
an		
· New . Mr. WARACCOURTER, Art. Incharger		Canceline

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

3-31

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

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

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

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

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

Figure 3.37 S Input Composition for Stream: Prop Dxide × Composition Basis © Mole Fractions 1.0000 0.0000 0.0000 3dio C Mass Fractions C Liq Yolume Fractions C Mole Flows C Mase Flows ← Lig Volume Flowe Composition Controls Erase Normalize Cancel Total 1.0000 OK.

composition is now defined for this stream.

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

16. Click the Normalize button to force the other values to zero. The

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

Name	Prop Dxide	** New **	
Vapour Fraction	0.0000		
Temperature (F)	75.00		
Pressure (psia)	16,17		
Molar Flow (Ibmole/hr)	150.0	1	
Mass Flow (lb/hr)	8712		
Liquid Volume Flow [USGPM]	20.83		
Heat Flow (Btu/hr)	-7.804e+006		
Walantal Strange Com	witche Energy Sh	ame Utat Dos	1000 CAN

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



Material Stream Icon

#### Adding Another Stream

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

18. To add the second feed stream, do any one of the following:

- Press F11.
- From the Flowsheet menu, select Add Stream.
- Double-click the Material Stream icon on the Object Palette.
- Click the Material Stream icon on the Object Palette, then click the Palette's Add Object button.

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

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

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

Worksheet		
	Stieam Name	Water Feet
Conditions	Vapour / Phase Fraction	<emply;< td=""></emply;<>
5	Temperature [F]	75,00
Properties	Pressure (psia)	16,170
Composition	Molar Flow (Ibmole/hr)	<empty:< td=""></empty:<>
K Value User Variables Notes	Mass How [ID/In]	<empty:< td=""></empty:<>
	Std Ideal Lig Vol Flow [USI3PM]	<empty)< td=""></empty)<>
	Molar Enchalpy (Btu/Ibmole)	(empty)
	Molar Entropy (Bitu/Dinole-F)	<empty)< td=""></empty)<>
	THEAT FLOW [BULLTY]	(empty)
ost ir arameters	Lid voi now (esto Lond (barrel/day)	<empty:< td=""></empty:<>
		13-33519-1
Worksheet []	Allachments Dunamics	
Worksheet	Attachments Dynamics	

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

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

Worksheet		Mole Fractions
Conditions	12C30xide 12-C3diol 14-20	A complyation of the second
Properties Composition		
K Value	· · · ·	
User Variables Notes		
Cost Parameters	Tota	J 0.00000
,	Egit Ed	it Properties Basis
Worksheet	tlachments Dynamics	area glughtan an an Aristo da a

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

and the second		
	CompMassFlow	Composition Basis
12C30xade	(empty)	C. Mole Fractions
12-1-3001		- C Mass Fractions
neu	11000.0000	C Lin Volume Fractions
Contraction of the second s		- Fed Transie & Grant a
	* (***********************************	C Mole Flows
a . e i sa co a standa de la state		G Mgss Flows
2. · · · · · · · · · · · · · · · · · · ·		C Lin Makana Shuus
		· Log Forming Fights
		Comparison Controls
		Erase
177 - 7 L		) <del>( ) ( ) ( ) ( ) ( ) ( ) ( ) ( ) ( ) </del>
- PAPERPROT		Normalize
Contraction of the		Bostowe - Barrier - Barrier
		and the second
4	1	

For the current Composition Basis setting, you want to enter the stream composition on a mass flow basis. 26. Since this stream has no other components, click the **Normalize** button. The other component mass flows are forced to zero.

🍕 Input Composition for Stream: Water Feed				
	CompMassFlow	Composition Basis		
12030 xcte	0.0000	C Mole Fractions		
12-C3diol	0.0000	C Mass Fractions		
M20	11000.0000	C Hard and Charles		
2 27.7 0		······································		
inging of the second	12 1. 1944, " an once a sub-transformer to the transformer to the second second second second second second sec	- C Mole Flows		
Y		G Mges Flows		
	10110 D011 1000 000000 0 D 10000000000	- C Lin Volume Bour		
<u>7</u>				
	A	Composition Controls		
A STREET, STORE				
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1		Normeige		
1 177	· · · · · · · · · · · · · · · · · · ·			
		Coccel		

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

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

Worksheet			weaus Phase
Continue	12030xide	00	0.0000
	H20	lo lo	1100
mopernes			
Composition			
K Value			**************************************
User Variables			
Notes		y Prestores	
Cost Paramaters	Total 1100.00000 lb/hv		
	Egit Edit	Properties	Basja

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

- 28. Click the Conditions page to view the calculated stream properties. You can display the properties of all phases by resizing the property view
- 29. Place the cursor over the right border of the view. The cursor changes to a double-ended sizing arrow.
- 30. With the sizing arrow visible, click and drag to the right until the horizontal scroll bar disappears, making the entire table visible.

Conditions         Vapour / Phase Fraction         0.00000         1.000           Processies         75.000         75.00         75.00           Processies         16.170         16.170         16.170           Composition         Molar Flow (Emole/hs)         61.060         61.0           K Value         Std (doed Liq V4 Flow [BSGPM]         2.2013         2.20           User Variables         Molar Entrably [Btu/Bmole]         -1.225e+005         1.225e+005           Notes         Molar Entrably [Btu/Bmole]         -1.4393         1.43           Heart Flow [Btu/Duncie-F]         1.4939         1.43           Heart Flow [Btu/Duncie-F]         -7.4013e+0C         7.4013e+1C           Cost Parameters         Liq Vol Flow @Std Cond [barel/day]         74.251         74.2	Worksheet	Stream Name	Water Feed	Aqueous Phase
Conditions         Temperature [F]         75.000         75.0           Properties         Pressure [psa]         16.170         16.1           Composition         Molar Flow [bnochrs]         61.080         61.080         61.080           K Value         Std Ideal Lis Vol Flow [LISGPM]         2.2013         2.20           User Variables         Molar Entrapy [But/Broole)         -1.225e-005         -1.225e-005           Notes         Favo [But/Broole)         -1.225e-005         -1.225e-005           Notes         Hear Flow [But/Broole)         -1.225e-005         -1.225e-005           Notes         Hear Flow [But/Broole)         -1.225e-005         -7.4013e-oc           Notes         Hear Flow [But/Broole)         -7.4013e-oc         -7.4013e-oc           Log Voi Flow @Std Cond [banel/dey]         74.251         74.2         Fluid Package	Conditions	Vapour / Phase Fraction	0.00000	1.0000
Properties         Pressure (psis)         16.170         16.1           Composition         Molar Flow (Bronderhy)         61.050         61.0           K Value         Std Ideal Liq Vol Flow (LISGPM)         2.2013         2.20           User Variables         Molar Entracy (Btu/Donole - T)         -1.225e+00         -1.225e+00           Notes         Hoar Entracy (Btu/Donole - T)         1.4393         1.43           Notes         Line (Btu/Pa)         -7.4813e+06         -7.4813e+10           Cost Parameters         Liq Vol Flow @Std Cond (Dansi/day)         74.251         74.2		Temperature [F]	75.800	75.00
Composition         Molar Flow (Bonderhy):         61,060         61.0           K Value         Ski lideal Liq Val Flow (BSGPM)         1100.0         1100           K Value         Ski lideal Liq Val Flow (BSGPM)         2.2013         2.20           User Variables         Molar Entratog (Btu/Donole)         -1.225e+005         1.225e+005           Notes         Molar Entratog (Btu/Donole-F)         1.4989         1.43           Heat Flow (Burkhal)         -7.4013e+005         -7.4013e+005         -7.4013e+005           Cost Parameters         Liq Vol Flow @Std Cond [banel/day]         74.251         74.2           Fluid Package         Basis-1	Properties	Pressure (psia)	16.170	15.17
Mass Flow [b/fv]         1100.0         1100.0           K Value         Sid Ideal Lig Vol Flow [B/SGPM]         2.2013         2.20           User Variables         Molar Entrador [But/Dimole]         -1.225e-005         -1.225e-005           Notes         Hear Flow [But/Dimole]         -1.235e-005         -7.403e-05           Lig Vol Flow (But/Dimole)         -7.403         -7.403           Lost Parameters         Lig Vol Flow (@Std Cond [bansl/deg/]         74.251           Fluid Package         Basis-1	Composition	Molar Flow (Ibmole/hr)	61,060	61.06
K Value         Std Ideal Lig Vol Flow [USGPM]         2.2013         2.20           User Variables         Molar Enthalpy [Btu/Tomole)         -1.225e+005         -1.225e+005           Notes         Molar Enthalpy [Btu/Tomole)         -1.225e+005         -1.225e+005           Notes         Heat Finous [Btu/Tomole-F]         1.4939         1.434           Cost Parameters         Lig Vol Flow @Std Cond [barrel/day]         -7.4913e+06         -7.4913e+           Fluid Package         Bosis-1         -74.251         74.2		Mass Flow [b/hr]	1100.0	1100.0
User Variables         Molar Enthalog [But/Donole]         -1.225e-00           Notes         -1.4389         1.4389           Notes         Heat Funday [But/Donole-T]         1.4389           Los Parameters         Lig Vol Flow @Std Cond [Danel/day]         -7.4013e-06           Fluid Package         Paste-1	KValue	Std Ideal Liq Vol Flow [USGPM]	2.2013	2.201
Notes Notes Heat Flow [Blut/bmole-F] 1.4999 1.49 Heat Flow [Blut/bmole-F] Cost Parameters Liq Vol Flow @Std Cond [barrel/day] 74.251 74.2 Fluid Package Pasis-1	User Variables	Molar Enthalpy [Btu/Ibmole]	-1.225e+005	-1.225e+00
Hear Flow [Blu/hs]         -7.4913e+06         -7.4913e+06           Cost Parameters         Liq Vol Flow @Std Cond [banel/day]         74.251         74.2           Fluid Package         Basise 1         Basise 1         Basise 1	Notes	Molar Entropy [Btu/Ibmole-F]	1.4989	1.498
Cost Parameters Liq Vol Fow @Std Cond [barrel/day] 74.251 74.2 Fluid Package Boste 1	1008	Heat Flow [Blu/hr]	-7.4913e+06	-7.4813e+0
Fuid Package Basis 1	Cost Parameters	Liq Vol Flow @6td Cond [barrel/day]	74.251	74.25
		Fluid Package	B934\$-J	
	1994 - A.	/		anga anan <b>assa a</b> ga at as ta ta banya, <b>ma</b> sa
			. Ere	

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

- In this case, the aqueous phase is identical to the overall phase.
- 31. Close the Water Feed property view to return to the Workbook.



Sizing Arrow Icon
## **Installing Unit Operations**

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

#### Installing the Mixer

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

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

* UnitOps - Case (Main)	
Categories	Ayalable Unit Operations
C All Unit Ops	Heater A
C Vesselt	Hif Alkylation
C Heat Transfer Equipment	Hydrocracker
C Rotating Equipment	Hydrocyclone
C Piping Equipment	LNG
C Solida Handling	MassBal SubFlowsheet
C Reactors	Mixer
Prebuit Columns	N/D Historiaalas
C Short Cut Columns	Perametric Unit Operation
C Sub-Flowsheets	PiD Controller
C Logicals	Proe Segment
C Extensions	Pum
C User Ops	Repoiled Absorber
C Electrolyte Equipment	Recycle
C Belinen One	Refinery Assay Fixer

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



Workbook Icon

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

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

#### The property view for the Mixer appears.



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

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

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

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

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

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

	. st	- AND		IX-100	Name M	esign	Desi
1.00	1			المنافقة المنافقة	- 709999 - 1383	sclions	Connecti
	tut.	ai 61		N		olova	Parameter
	377 		2			anables	User Variai
				<u>→</u> //			TTURES
e i	ने े			<b></b>	injets		
		de ar	FlidPer		Prop Oxide		122.2
Ċ,	J		Basis-1	-	Water Feed		and the second sec
	3		Oyliet Fluid Peo Basis-1	L∕ ¶	Injets 2 Prop Quide Water Feed		

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

			. 0 ×
Design Connections Parameters User Variables Notes	Nane MK-100	$\sum_{i=1}^{n}$	
	Prop Oxide Water Feed << Stream >>	Oglet Mixer Out Fuid Package Basis-1	

Alternatively, you can connect the stream by typing the exact stream name in the <<Stream>> cell, then pressing ENTER. The status indicator displays a green **OK**, indicating that the operation and attached streams are completely calculated. The Connections page is now complete.

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

Design	
Connections	
Parameters	e 🗠 🖓 a construction and a construction of the construction of t
User Variables	. [ ] <del>                                    </del>
Notes	
	Putomatic Pressure Assignment
	i (* Sei Oydet to Lowest inie

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

Workshoet	Name	Prop Oxide	Water Feed	Mixer Out
Conditions	Vapour	0.0000	0.0000	0.0000
- a particulo ( )	Temperature [F]	75.00	75.00	75.00
Properties	Pressue [psia]	16.17	16.17	16.17
Composition	Nolar Flow [Ibmole/hr]	150.0	610.6	760.6
PF Spece	Mass Flow (b/hr)	8712	1.100e+004	1,971e+004
	Std Ideal Lig Vol Flow [USGPM]	20.83	22.01	42.84
1	Molar Enthalpy (Btu/Ibmole)	-5.203e+004	1.225e+005	-1.066e+005
i min ti	Molar Entropy [Btu/Ibmole F]	-5.768	1.499	0.8824
	Heat Flow (Btu/hr)	-7.804e+006	-7.481e+007	-8.262e+007

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

HYSYS has calculated the outlet stream by combining the two inlets and flashing the mixture at the lowest pressure of the inlet streams. In this case, both inlets have the same pressure (16.17 psia), so the outlet stream is set to 16.17 psia. 16. In the Workbook, click the **Unit Ops** tab. The new operation appears in the table.

Name	Object Type	lciet	Outlet	Ignored Calc. Leve
MIX-100	Mixer	Prop Oxide Water Feed	Mixer Out	F 50
Yiew UnitOp	Add UnitOp			Delete UnitOp
Material Streams	Compositions En	angy Streams Unit Ope		

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

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

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

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

### Workbook Features

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

#### Accessing Unit Operations from the Workbook

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

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

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

Name	1 F	hop Oxide	Water Feed	Mixer Out
Vapour Fraction		0.0000	0.0000	0.0000
Temperature [F]	· · · · · · · · · · · · · · · · · · ·	75.00	75.00	75.00
Pressure (psia)		16.17	16.17	16.17
Molar Flow [lbmole/hr]		150.0	610.6	760.6
Mass Flow [b/h/]		8712	1,100e+004	1.971e+004
Liquid Volume Flow (USC	PM]	20.83	22.01	42.84
Heat Flow [Btu/hr]	-7.	904e+006	-7.481e+007	-8.262e+007
Name	1	** New **		-
Material Streams	Compositions	Energy S	treams Unit Op	s j

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

#### Adding a Tab to the Workbook

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

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

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

The Workbook Setup view appears.

🕷 Setup				
Workbook Tabs		Tab Contents	ۋىشىد 📄	
Material Streams	Add	Object		the second second
Energy Streams	السيبيية	Name: Material Streams		g Order
Unit Ops	Uelete	Tupe: Material St	mam	New Tupe
		Yariables		· · · · · · · · · · · · · · · · · · ·
1. 1. 1. 1.		Variable	Format	Lise Set
		Vapour Fraction	1.4 fixed	
		Temperature	4 sig fig	Add.
AN THE REAL PROPERTY.		Pressure	4 sig fig	
11	- # 1	Molar Flow	4 sig fig	Delete
1 이외 : 20 전 영향 분기		Mass Flow	4 sig fig	
14 No. 14		Liquid Volume Flow	4 sig fig	Forwar"
	그 안 집 안가 가 많이	Heat Flow	4 sia ha	

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

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

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



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

Object	The second s
فستستعد فتقت فتحصب فالتشرخ المراجع المراجع	
Name P.T.Flow	Order
Contraction of the second s	1 21 5 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
Type: Material Stream	New Type
have a supervised and the second s	
⊻ariables	
Variable Format	Use Set.
Vapour Fraction 1.4 fixe	d be
Temperature 4 sig f	ig Add
Pressure 4 sig f	ig
MolarFlow 4 sig f	ig <b>Dølete</b>
Mass Flow 4 sig f	9
Std Ideal Lig Vol Flow 4 sig f	ig <b>Loima</b> i
Heat Flow 4 sig f	ig

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

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

Setup	and the second s	7.C.	e an seathan	aller i anne saide
Workbook Taos	- Add.	(Object	<u></u>	
P,T Flow Compositions		Name: P.T.Flow	. Witter in succession	Qider
Energy Streams		Type: Material SI	neen	New Lype .
and the second		l:		<u></u>
		Tarres		
		Yanabie Temperature	4 sig lig	Usa Set
	· · · · · · · · · · · · ·	Piessure	4 sig fig	édd
· · · ·		Std Ideal Lig Vol Flow	4 sig lig	Delete
				Format
			***	

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

	water reed i	Miser Dut	
75.00	75.00	75.00	-
16.17	16.17	16.17	1
150.0	610.6	760.6	11
20.83	22.01	42.84	iii iii
** New **		1	
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			Ŀ.
			-
			í,
	75.00 16.17 150.0 20.83 "New "	75 00 75 00 16.17 16.17 1500 5106 20.83 22.01 ** New **	7500 7500 7500 16.17 16.17 16.17 150.0 510.6 510.6 760.6 20.83 22.01 42.84 ** New **

12. Save the case.

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



# 3.2.7 Installing Equipment on the PFD

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

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



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

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

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

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



Fly-by information



Size Icon



Zoom Out 25%



+

Display Entire PFD

Zoom In 25%

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

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

## **Calculation Status**

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

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

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

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

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



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

## Installing the Reactor

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

- 1. Ensure that the Object Palette is displayed; if it is not, press F4.
- 2. You will add the CSTR to the right of the Mixer, so if you need to make some empty space available in the PFD, scroll to the right using the horizontal scroll bar.
- 3. In the Object Palette, click the CSTR icon.
- 4. Position the cursor in the PFD to the right of the Mixer Out stream. The cursor changes to a special cursor with a plus (+) symbol attached to it. The symbol indicates the location of the operation icon.



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

Attach Mode Icon

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

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

## Attaching Streams to the Reactor

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



- 3. With the pop-up 'Out' visible, click and hold the mouse button. The transparent box becomes solid black, indicating that you are beginning a connection.
- 4. Move the cursor toward the left (inlet) side of the CSTR-100 icon. A line appears between the Mixer Out stream icon and the cursor, and multiple connection points (blue) appear at the Reactor inlet.
- 5. Place the cursor near a connection point until a solid white box appears at the cursor tip, indicating an acceptable end point for the connection.



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

3-50



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



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

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



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

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

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

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

## **Completing the Reactor Specifications**

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



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

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

Design					
Connections				- 1 m	÷, te
User Variables	na P	1.0000 osi	$\Theta'_{*}$	Single Erlate	sel produce i pro-
Notes	Seven 1		K Ke	mpty>	<u> </u>
	· · · · · · · · · · · · · · · · · · ·		IV   14	uid Volume	
			1/ \ [ <sup>6</sup>	mply>	
	C Heating	Cooling	<u>E</u>	yid Lovel	
	Duty		<u>م</u> ا کے	00× 	

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

	minimized as a constraint of the second seco		- I
1Set Set-1	Ecoction	n Ran-1 🚬	1
s C Stoichiometry	C Baus	View Reaction	
ent			1
Component	Mole Wt.	Stoich Coeff	
H20	18.015	-1.000	с с
12C3Oxide	58.080	-1.000	11 : .
12-C3diol	76.096	1.000	
"Add Comp"			
1		1	136 166
a an gin the <b>B</b> a	dance Error	0.00000	
<b>J</b> Ri	saction Heat (25°C)	-3.9e+04 Stu/Ibmole	
			N
	cs C Stoichiometry etry Component H20 12C30/ide 12C30/ide 12C30/ide 12C3d/id	cs & Stoichingetry C gasis etry Component Mole W1 H2D 19.015 12C30.vide 58.080 12C30.vide 58.080 12C3.did 76.095 "Add Comp" Balance Error F Rescition Heat (25°C)	Cs         C Stoichingety         C gasis         Yew Reaction           ety         Considerent         Mole Wt.         Stoich Coeff           12C30.vide         58.080         -1.000           12C30.vide         58.080         -1.000           12C30.vide         58.080         -1.000           "Add Comp"

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

8. Click the Dynamics tab, then select the Specs page.

----

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

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C Initiation From Products	The seal block and 1671	10.000
C Dry Startup	Vessel Diameter (R)	6,194
C Initialize From User	Height [R]	9.291
Jell Hold to Car	Liq Volume Percent [%]	85.00
manneds	Level Calculator	Vertical cylinder
🔽 Lag Ran Temperature	Fraction Calculator U	se levels and nozzles
F Enable Explicit Reaction	) Calculations	
-Dunamic Specifications		na har gandal angan dan gan dan dan dan dan dan dan dan dan dan d
Fand Data P [on]	1 0.000	
Versel Pressure (psia)	16.17	F
and the second	المرميل المرسمة بالإيضائية المحمد المراسي أيمي	humphrough and the second second
A MARKET AND A MARKET	the stand of the second se	1
	C Initiatize From Products C Dry Startup C Initiatize From User Init Hold Ip ↓ F Lag Ran Temperature F Enable Explicit Reaction Dynamic Specifications Feed Deka P [psi]	G     Initialize From Products     Vessel Volume [f3]       C     Dgp Startup     Vessel Volume [f3]       C     Jptialize From User     Height [10]       Initialize From User     Height [10]       Init Hold 1p     Liq Volume Percent [21]       F     Lag Ran Temperature       Fraction Calculator     U       IF     Enable Explicit Reaction Calculator       Dignamic Specifications     0.0000       Vessel Pressure [psie]     16.17

11. Click on the Worksheet tab.

	The state of the second second second	Minet Oct	Desetes Desete	Baseley March 1	n marken in the second
Workshow	Verner	Misidi Uut	0.0000	1 0000	Cutian
Conditions	Temperahas (E)	25.00	(emphi)		(empty)
President .	Press ve Instal	16 17	1617	16 17	(emply)
	Moder Flow (Innote Arc)	760.6	(emotio)	(amplu)	(empty)
Composition	Mass Flow Ib/hil	1.971e+004	(emntu)	(empty)	cemptus
PF Specs	Std Ideal Lip Vol Flow JUSGPM	42.84	(emoty)	<emoty></emoty>	(empty)
1. M. 18 19	Molar Enthaloy (Btu/Ibmole)	-1.086e+005	(empty)	(emptu)	(empty)
	Molar Entropy [Btu/tomole-F]	0.8824	<empty></empty>	(empty)	<empty></empty>
· · · · · · · · · · · · · · · · · · ·	Heat Flow (Blu/hr)	-8 262e+007	<empty></empty>	<empty></empty>	<empty></empty>
and the second sec			Contraction of Condition of	and the second	a contraction and a second
19 <del>1</del> 8					
			1		
			1		
1 The Street	C. C. M. S. Marshell, C. M. M. W.				
一、学习 認知 天 由此		·		1	

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

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

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

Reactor - Set-1				the second	للع کر کہ
Worksheet	Name	Mixer Out	Reactor Prods	Reactor Vent	Coolan
n h:	Vapour	0.0000	0.0000	1.0000	<empty:< td=""></empty:<>
Londitions	Temperature (F)	75.00	75.00	75.00	(empty)
Properties	Pressure (psia)	16.17	16.17	16.17	<empty)< td=""></empty)<>
Companyion	Molar Flow [ibmole/hr]	760.6	700.2	0.0000	<empty:< td=""></empty:<>
Composition	Mass Flow [b/hr]	1.971e+004	1.971e+004	0.0000	<empty)< td=""></empty)<>
PF Specs	Std Ideal Liq Vol Flow [USGPM]	42.84	41.10	0.0000	<empty)< td=""></empty)<>
	Molar Enthalpy [Btu/Ibmole]	-1 086e+005	-1.214e+005	-5.030e+004	<empty:< td=""></empty:<>
	Molar Entropy (Btu/bmole F)	0.8824	0.6769	20.68	<empty:< td=""></empty:<>
	Heat Flow [Btu/hr]	-8.262e+007	-8.499e+007	0.0000	-2.372e+006
Design Reacti	ons Rating Worksheet Dynamic	 •			

There is no phase change in the Reactor under isothermal conditions since the flow of the vapour product stream Reactor Vent is zero. In addition, the required cooling duty has been calculated and is represented by the Heat Flow of stream Coolant. The next step is to examine the Reactor conversion as a function of temperature. 13. Click the **Reactions** tab, then select the **Results** page. The conversion appears in the Reactor Results Summary table.

Reactions	Reaction Results S	umay			T.
Dolais Rosults	Astr.1	Act X Cnv 40.30	Bese Comp 12C3Oxide	Aven Extent 60.45	
Level 2					
			1995 - 1975 - 1975 - 1975 - 1977 - 19		

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

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



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

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

Reaction Results Summary Peeption Egenta Act. 2 Cmy Base Comp Ron Extent	Figure 3.72			
Act. % Crw, Base Comp. Rish Extent	Reaction Results Sur	nmaiy C Reactio	n Balance	
		Act & Criv,	Base Comp	Ren Extent

19. Close the Reactor property view.

## Installing the Column

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

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

Condenser Energy Stream		<u> </u>	Condense	•	
Column Name T-100		$\rightarrow (2)$	0 C Patha	Dynd Out	M
	6	$\rightarrow$	T rul	B×]	
Iniel Streams		and alter of	, ⊂ Water	Drew	
Stream Inlet Stag	e T		Dolinoal Side (		
:< Stream >>			Stream	I Type   D	raw Stage
A T L LOT & SMARIN			Stream >>		
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이는 말라고 있는 것을 같이 없다.	<u></u>	Re Re	poiler Energy Stream	n	Contractor
			and the second of	Bottoma Li	auid Outlet
Ctore blumbering	<u> </u>	nei			7
College Manuella		<u>~~(&lt;)</u> _		all an 14	



Distillation Column Icon

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

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

- When you install a column using a pre-built template, HYSYS supplies certain default information, such as the number of stages. The **Numb of Stages** field contains **10** (default number of stages). Note the following:
  - These are theoretical stages, as the HYSYS default stage efficiency is one.
  - The Condenser and Reboiler are considered separate from the other stages, and are not included in the Num of Stages field.

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

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



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

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



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

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

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

- The Flow Basis applies to the Vapour Rate, so leave it at the default of Molar.
- 16. In the Vapour Rate field, enter 0 lbmole/hr. In the Reflux Ratio field, enter 1.0.

S Distillation C	olumn Input Exp	eil			- In comm	×
		Æ	-Q-[	<b>-</b> <sup>-</sup> <sup>4</sup>	xxur Rate  00000	<b></b>
12.21 17.22 17.22	1.1.1.1.1.1.1.1.1.1.1.1.1.1.1.1.1.1.1.	-	Reflux Ratio		ow Basis Molar	
	Q					
	24. <sup>3</sup> 74 - 4 3 A ily					
			-65-			en e

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

Design	Optio	nal Check	<b>.</b>	میں ایس	in the second	Profile		<b>Million 14</b>	y Por New York	ταρ
Connections		out Summ	<u>.</u>	View la	vital Estimates	<b></b>	\$000			
Monitor	Liter.	Step	Equi	brium	Heat / Spec	C lent		2 2 8		
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	Ovto	IVap Rati			1.0000 lbmole/hr	7.94e-01	3 0.0000	ম	9	7
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	<b>k</b>	Ymm		dd Spec	. Group	Active	Upgate Inactive	Degn	nes of Free	odom 10
	I. Innerstand					Transie and the second				

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

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

#### Adding a Column Specification

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

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

Name	Comp Fraction
Stage	<< Stage >>
Flow Basis	Mole Fraction
Phese	Liquid
Spec Value	(emply)
Components	<< Component>>
et 1	
	a al company and a second

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

State	M2U Fraction					
Plane Basis Phase Spec Value Components	5_Main TS 6_Main TS 7_Main TS 8_Main TS 10_Main TS 10_Main TS					
Target Type	(* Sliege					

Column Specification Types
Column Cold Properties Spec
Column Component Flow
Column Component Fraction
Column Component Ratio
Column Component Recovery
Column Cut Point
Column Draw Rate
Column DT (Heater/Cooler) Spec
Column Dt Spec
Column Duty
Column Duty Ratio
Column Food Ratio
Column Gap Cut Point
Lolumn Liquid Flow
Coumn Physical Properties Spec
Column Pump Around
Calumn Hebbi Hado Spec
Column Belly Feed Batis Sone
Column Bellux Fraction Spec
Column Reflex Ratio
Column Tee Solt Spec
Column Temperature
Column Transport Properties Spec
Column User Property Spec
Column Vapour Flow
Column Vapour Fraction Spec
Column Vapour Pressure Spec
and a second second
0.00 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2

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

Compilation opposition	
Name	H20 Fraction
Stage	Reboiler
Flow Basis	Mole Fraction
Spec Value	5.000e-003
Components:	H20
	<< Component >>
Target Type	Stream 🤄 Stage

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

Design	opiolaci	ecka		Y	Pione	Tellet	abri 16. Tin	Persona and a	Top
Connections	Input St	mary	VIOW II	nial Estimates		9000			
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opecs ournmary		naniarini ana				2033		-	
Subcooling		· · · · · ·			······ }	1000		6 8	10 12
Notes	Consilionio	<b></b>		27 - C	Lanna and the second				
	- Coprocession		1 Sp	cified Value	Current Value	WE Error	Active	Estimate	Cunert
	Ovhd Vap	Rate		0.0000 lbmole/hr	7.94e-013	0.0000	9	9	9
	Reflux Rati	0		1.000	(empty)	(empty)	A	9	7
	H20 Fracti	on i		5.000e-003	<empty></empty>	<emply></emply>	<b>v</b>	A	<b>ਸ</b>
	Distillate R.	de .		(empty)	(empty)	<empty></empty>	Г	R	<u> </u>
	Reflat Rat			<emply></emply>	<empty></empty>	<emply></emply>	<u> </u>	<u>P</u>	<u> </u>
	Hums Frod	Hale		(emply)	<empty></empty>	<ampty></ampty>	<u> </u>	L. K	
	] <b>.</b>				i	······································		L	
·	View	. [	Add Spec,	Gioup/	Clive Upp	ats inactive	Dece	ins of Fran	dom 0

If you want to view the entire Specifications table, re-size the view by clicking and dragging its bottom border. HYSYS automatically made the new specification Active when you created it. The Degrees of Freedom has returned to zero, so the column is ready to be calculated.

#### Running the Column

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

Dexign	Optional Checks	17 8 7 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	Profile	Tumper	WA W. TA	y Bos Mon Main 7	( <b>(p</b> )
Connections	Input Summary	View Initial Estimates					
Monitor	C Day 1 Chan 1	a Marine Unat Dealer	C Temp				7
		0.050935 0.224420	- C Press	360	1	1 17	
Spece	2 1.0000	0.031171 0.070670	C Flows	200		1	
Specs Summary	3 0.2500	0.002362 0.013733	1	200		+ +	
Subcooling	4 0.000	0.000003 0.0002672		150.0			
		Specified Value	Current Value	Wt. Error	Active	Estimate	Current
	Ovhd Vap Rate	0 0000 ibmole/hr	1.66e-005	0.0000	<u> </u>	P	<u> </u>
	Hellux Halio	1.000	1.00	-0.0000	M		
	Distillate Data	5.000e-003	2.010-003	u.uuus			
	Reflux Rate	(emply)	476	(emply)		6	
	Btms Prod Rate	<empty></empty>	143	<empty></empty>	r	ন	ř
	<u>}</u>	Add Spec. Gioup	Active Ups	ate inactive	Degr	bes of Freed	tom 0

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

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

Figure 3.83 Folumn: Tower / COL1\_Fluid Pkg: Basis-1 / UNIQUAC - Ideal Basis Reflux Ratio Rebail Ratio Performance 1.000 G Flows C Epergy · Mola C Mass ( Lig Yol Summary Column Profile noevaluze Pressure (psia) 15.00 Net Liouzd Net Vapour Not Feed Net Dia F 159.0 12.7 (bmole/hr) 475,785 Feeds/Products [lbmole/hr] (Ibmole/hr) ibmoie/h Condenser 475 79 Plots 212.2 \_\_Main TS \_\_Main TS \_\_Main TS 15.00 498.675 951.571 213.4 214.1 15.22 15.44 498.964 498.737 974.460 974.750 974.522 970.111 Main TS 215.2 15 67 494.326 \_Main TS \_Main TS 618.55 15.89 16.11 1188.80 220.9 222.0 1189.94 1046.04 Main TS Main TS 223.0 16.33 1183.75 231.0 16.56 1040.99 1082.20 9\_\_\_Main TS 10 Main TS 16.78 939.438 771.084 294.5 913.848 360.0 960.612 375.7 17.00 817.847 142.76 eboiler

Design Parameters Side Ops Rating Worksheet Performance Flowsheet Reactions Dynamics

Beset

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Ryn

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

Delete

Column Environment...

Accessing the Column Sub-flowsheet

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

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





Workbook Icon



Column Runner Icon

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



- When you are finished in the column environment, return to the 2. Main Flowsheet by clicking the Enter Parent Simulation Environment icon.
- 3. Open the PFD for the Main Flowsheet and select Auto Position All from the PFD menu. HYSYS arranges your PFD in a logical manner.



#### Moving Objects and Labels in a PFD

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

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

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



# 3.2.8 Viewing Results

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

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

• Workbook • Lase [Main]					
Name Name K.P	Prop Oxide	Water Feed	Mixer Out	Reactor Vent	-
Vapour Fraction	0.0000	0.0000	0.0000	1.0000	5
Comperature (F)	75.00	75.00	75.00	140.0	1
Pressure (psia)	16.17	16.17	16.17	16.17	Τ.
Molar Flow [Ibmole/hr]	150.0	610.6	760.6	0.0000	1.
Mass Flow (b/h)	8712	1.100e+004	1.971e+004	0.0000	] -
Liquid Volume Flow [USGPM]	20.83	22.01	42.84	0.0000	ļ,
Heat Flow [Btu/hr]	-7.804e+006	-7.481e+007	-8.262e+007	0.0000	
Name	Reactor Prods	Glycol	0vhdVap	RecyProds	
Apour Fraction	0.0000	0.0000	1.0000	0.0000	1
emperature [F]	140.0	375.7	159.0	153.0	þa.
Tessue [psia]	16.17	17.00	15.00	15 00	1.
Molar Flow [Ibmole/hr]	618.5	142.8	4.369e-005	475.8	1
Mass Flow (ID/hr)	1.971e+004	1.0826+004	2.006e-003	8890	l.
Jourd Volume Flow [USGPM]	38.75	20.78	4.7016-006	17.97	j
test Flow (Btu/hr) Meterial Streams PT.Fk Feeder8lock, Prop Dxide MIX-100	-8,714e+007	2.803e+007	2.534	-5,700e+007 ( b-Flowsheets e Only en Objects: 0	
test Flow (Btu/hr) Material Streams P.T.Fk FeederBlock, Prop Dikk	8.714e+007	2.903e+007	2 534	-5,700e+007 ( b-Flowsheets e Only en Objects: - 0	<u> </u>
teat Flow (Btu/hr) Material Streams P.T.Fk FeederBlock, Prop Didk MIX-100 Workbook Case (Main)	8.714e+007	-2.803e+007	2 534	-5,700e+007 ( b-Flowsheets e Only en Objects: 0	×
Heat Flow (Btu/hr) Material Streams P.T.Fk FeederBlock, Prop Oxide MIX-100 Workbook Case (Main) Name	8.714e+007	2.803e+007	2 534 Urit Ope Include Su Show Nam Number of Hidd	-5,700e+007 ( b Flowsheets e Only en Objects: 0 Fleactor Vent	×
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teat Flow (Btu/hr)  Material Streams P.T.Fk FeederBlock, Prop Dxide MD-100  Workbook Case (Main) Name: Comp Mole Flac (12:30,ade) Comp Mole Frac (12:30,ade)	8.714e+007   w Compositions Prop.Oxide 1.0000 0.0000	2.803e+007	2 534 Unit Op: Show Nam Number of Hidd Mixer Out 0 1972 0 0000	-5,700e+007 bFlowsheets e Only en Objects: 0 Reactor Vent 0.3911 0.0043	×
teat Flow (Btu/hr) Material Streams P.T.Fk FeederBlock, Prop Oxide MEX100 Workbook Cose (Main) Name Comp Mole Frac (12/30,ade) Comp Mole Frac (12/30,ade) Comp Mole Frac (12/30,ade) Comp Mole Frac (12/30,ade)	8.7146+007	2.803e+007   J Energy Streams Water Freed 0.0000 0.0000 1.0000	2 534 Unit Ope Include Su Show Nam Number of Hidd Miser Out 0.1972 0.0000 0.8028	-5,700e+007 - Flowsheets = Only = Objects - 0 - fc0 - fc	×
teat Flow (Bturk) Material Streams P.T.Fk FeederBlock, Prop Oxide MK-100 Workbook Case (Main) Name Comp Mole Frac (12C3Daide) Comp Mole Frac (12C3Daide) Comp Mole Frac (12C3daid) Comp Mole Frac (12C3daid) Name	8.714e+007 w Compositions Prop Oxide 1.0000 0.0000 Reactor Prods	2.803e+007     Energy Streams   Water Feed   0.0000   0.0000   0.0000   0.0000	2 534 Unit Opc Show Nam Number of Hidd Mixer Out 0.1972 0.0000 0.8028 0 vhdVap	-5,700+007 b Flowsheets e Dray en Objects - 0 -100 Reactor Vent 0,3911 0,0049 0,6040 RecyProds	×
teat Flow (Btu/hr) Material Streams P.T.Fk FeederBlock, Prop Oxide MIX-100 Workbook Cose (Moin) Name: Comp Mole Frac (12/C30/side) Comp Mole Frac (12/C30/side) Comp Mole Frac (12/C30/side)	-8.7146+007   	2.803e+007   J Energy Streams Water Feed 0.0000 0.0000 0.0000 Glycol 0.0000	-2.534	-5,700e+007 - Flowsheets e Only en Objects: 0 - 100 -	×
test Flow (Btu/hr) Material Streams P.T.Fk FeederBlock, Prop Oxide MEX100 Workbook Case (Main) Nams Comp Mole Frac (12/C30,ide) Comp Mole Frac (12/C30,ide)	8.7146+007	2.803e+007	-2.534 Unit Das 	-5,700+007 -5,700 -5,700	
teat Flow (Bturk) Material Streams P.T.Fk FeederBlock, Prop Oxide MK-100 Workbook Case (Main) Name Comp Mole Frac (12C3Disde) Comp Mole	8.714e+007 w Compositions Prop.Oxide 1.0000 0.0000 Reactor Prods 0.0129 0.2296 0.7575	2.803e+007     Energy Streams   Water Feed 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	-2.534 Unit Opc 	-5,700+007 -5,700+000+000+000+000+000+000+000+000+000	
teat Flow (Bturk) Material Streams P.T.Fk FeederBlock, Prop Dikk MIX-100 Workbook Gase (Main) Name Comp Mole Frac (12C3Q)// Comp Mole Frac (1	8.714e+007 Compositions Prop.Oxide 1.0000 0.0000 0.0000 Resolv Prods 0.0123 0.2296 0.7575 *** New ***	2.803e+007	-2.534 -2.534 -3.160 Dec -3.160 Dec -3	-5,700e+007 -Flowsheets e Only en Objects: 0 Reactor Vent 0,0043 0,0043 0,0043 0,0043 0,0043 0,0043 0,0043 0,0043 0,0043 0,0045 0,0000 0,98033 0,98030	×
test Flow (Btu/hr) Material Streams P.T.Fk Feeder6lock, Prop Oxide MIX-100 Workbook Case (Main) Name Comp Mole Frac (12C30,side) Comp Mole Frac (12C30,side)	8.7146+007 W Compositions Prop Dxide 1.0000 0.0000 0.0000 Resolution 0.0029 0.2286 0.7575 ** New **	2.803e+007	-2.534 Unit Dos Include Su Show Nam Nümber of Hidd Mixer Cut 0.1972 0.0000 0.8028 0.4040/spc 0.0000 0.3038	-5,700+007 -Flowsheets e Only e Only e Only e Only -ft -ft -ft -ft -ft -ft -ft -ft	
text Flow (Btu/hr) Material Streams P.T.Fk FeederBick, Prop Oxide MK-100 Workbook Cose (Main) Name Comp Mole Frac (12:30,sde) Comp Mole Frac (12:30,sde)	8.714e+007 w Compositions Prop Oxide 1.0000 0.0000 0.0000 Reactor Prods 0.01256 0.7575 ** New **	2.803e+007   J. Energy Streams Water Feed 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	-2.534 Unit Ope 	-5,700e+007 -Flowsheets e Only en Objects 0 -101 Reactor Vent 0.3911 0.0049 0.6040 RecyProds 0.0167 0.0000 0.9833	
teat Flow (Btur/hr) Material Streams P.T.Fic FeederBlock, Prop Diskt MIX-100 Workbook Case (Motin) Neme Comp Mole Frac (12C30,side) Comp Mole Frac (12C30,	8.714e+007	2.803e+007	-2.534	-5,700e+007 -Flowsheets en Objects: 0 Reactor Vent 0,0043 0,0043 0,0043 0,0043 0,0043 0,0043 0,0043 0,0043 0,0043 0,0043 0,0045 0,004	
test Flow (Btu/hr) Material Streams P.T.Fk Feeder6lock, Prop Oxide Mkx100 Workbook Cose (Main) Name Comp Mole Frac (12C30,ide) Comp Mol		2.803e+007	-2.534 Unit One Include Su Show Nam Nümber of Hidd Miser Out 0.1972 0.0000 0.8028 0.0000 0.8052 0.0000 0.3038 Unit Ose	-5,700+007 - Flowsheets e Only en Objects: 0 - [13] Reacior Vent 0.3911 0.0049 0.5040 RecyProds 0.0167 0.0000 0.9833	

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## Using the Object Navigator

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

To open the Navigator, do one of the following:

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

The Object Navigator view appears.

A Object Navigator			
Flowsheets.		perations	File
Case (Main) Tower (COL1	) MIX- Reac Town	100 xtor pr	C All C Streams C UnitOps C Lonicals
			C Custom Setup Custom

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

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

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

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



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

You can start or end the search string with an asterisk (\*), which acts as a wildcard character. This lets you find multiple objects with one search. For example, searching for VLV\* will open the property view for all objects with VLV at the beginning of their name. 3-67

### Using the Databook

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

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

The Databook view appears.

≪ Datalio	ok Marina andreas	- * · · · ·	 	- 10.21			
Ayailable Object	Data Enlines	Variable	TAN.	gringer (* 1997) Eller			و سامین اور تاریخ
	9					in Kolt. Almeri	
		- Khat			, v	Deis	
n Arthur	12, 2447 (*). 11 - T						1
							and a

To edit any of the Objects in the Databook:

- 1. Select the Object you want to edit.
- 2. Click the Edit button.
- The first task is to add key variables to the Databook. For this example, the effects of the Reactor temperature on the Reactor cooling duty and Glycol production rate will be examined.
- 3. On the Variables tab, click the Insert button. The Variable Navigator appears.
- 4. In the Object Filter group, select the **UnitOps** radio button. The Object list is filtered to show unit operations only.
- 5. In the Object list, select Reactor. The variables available for the Reactor object appear in the Variable list.

The Variable Navigator is used extensively in HYSYS for locating and selecting variables. The Navigator operates in a left-to-right manner—the selected Flowsheet determines the Object list, the chosen Object dictates the Variable list, and the selected Variable determines whether any Variable Specifics are available. 6. In the Variable list, select Vessel Temperature. Vessel Temperature appears in the Variable Description field. You can edit the default variable description.

Variable Navigator				
Flowsheet	Object	Yariabla	Valiable Specifice	#W.W.#
Case (Main)	MIX-100	Vapour Level		OK
Tower (COL1)	Reactor	Vapour Mass Flow		
이 나는 동안이에	1 Buon	Vapour Mole Fracti		Object Filter
		Vapour Moles		CAL
1967 C		Vapour Volume		C Streams
1 Land March 1	We the first section of the	Vapour Volume Flor	18 N 18	C UniOps
Navigator Scope	d i the statistication	Vessel Geometry (C		C Logicals
G Eloupheel	Leg when	Vessel Length or H		C ColumnCos
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		Vessel Temperature		LUSOR
and the second secon		Volume, Fixed Dide		
A MARKENS		Volume, Sorted by F		1. 1.

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

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Object	Va	niable: 🔬 🗧	1. A. S.				e is Altar e at	1
Reactor	Re	lector Temp	an crimer				di 👘	
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			a de la compañía de l Compañía de la compañía	1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 - 1997 -				ľ

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

11. In the Variable list, select Heat Flow.

Flowsheet	Dhject	Yanabia	Valiable Specifics	
ase (Main) Tower (COL1)	CendDuty Coolant Gilycol	Heat Flow Dveral UA Power	ST Y ST	<u>OK</u>
	Mixer Out OvhdVap Prop Oxide Bastor Pode	Temperature Approach User Variables Utility flow rate		C All C Streams
lavigator Scope	Reactor Veni RebDuty RecyPtode	Utility Fluid Holdup Utility Inlet Temp Utility maximum flow rat		C UnitOps C Logicals
Cate Basia	Water Foed	Utility minimum flow rate Utility Outlet Temp		Custom
Flowsheet Cere Basis Uliky	ReciPiods William Feed	Utility maximum flow rat Utility minimum flow rat Utility Outlet Temp		Custon

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



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

14. Click the Process Data Tables tab.

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

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

Available Process Data Tables-		ividual Process Data	Selection	
ProcDate1 Vie	w.   P1	ocess Date Table	ProcData1	
		Object	Variable	Show
L		Reactor	Reactor Temp	Г
De		Coolant	Cooling Duly	Г
11		Giycoi	Glycol Production	Г
Set Set	tup: 1			
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	200 - 10 <b>-</b> -			
	13 年間	s second and a second	المراجع والمراجع والمراجعين	1

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

Figure 3.95		
Individual Process D	ata Selection	
Process Data Table	Key Variables	
Object	Variable	Show
Reactor	Reactor Temp	
Coolant	Cooling Duty	<b>v</b>
Glycol	Glycol Production	
I		

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

Object Variable Value Ur Reactor Reactor Temp 140.0		TO 12 27000
Reactor Reactor Temp 140.0	uts 🔤	
Contract Contract Duty 1 520a 0000	F	F
Coolark Coolary Duy 4 3208-000	Btu/hr	/hr
Giycol Gilycol Production 713.4 ba	rei/day	ley

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

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

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

20. Click the Data Recorder tab in the Databook.

- Uatabook	- 14- 14- <u>1</u> -14- 14- "%	o na ser a com		
Available Scenarios	Data Re	scorder Data Selei	ction	
	Dutten	t Scepario		
<b>B</b> QA		biect	Variable	Include
Distance -		Coolant	Cooling Duty	<b>     </b>
Deciel		Glycol	Glycol Production	
Available Gootha	The second se			
C Table	· · · · · · · · · · · · · · · · · · ·			
C Graph	\$\$ <b>}</b>			

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

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

Include
N R
2

3-72
📽 New Solved St 🔀	]
Name for New State	
State 1	
Дĸ	

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

State	Base Case				T		
Reactor Temp [F]	140.0				I	I	
Cooling Duty [Etu/hr]	4.520e+00E						
<b>Glucol Production (ba</b>	713.4				1		
a such the set of the							
1 S. L. S. L. S. S. S. Sandard S. P.		NALL ALL MAL MARTING	en anten san tana sasan di sa	<ul> <li>CONTRACTOR CONTRACTOR</li> </ul>	-		
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78							
					4		
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Now you can make the necessary flowsheet changes and these current values remain as a permanent record in the Data Recorder unless you choose to erase them.

- 26. Click the Minimize icon on the Data Recorder view.
- 27. Click the **Restore Up** icon **1** on the Key Variables Data title bar to restore the view to its regular size.

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

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



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

Object	Variable	Value	Units	Worksheet	[Stream Name	Reactor Proc
Reactor	ReactorTemp	140.0	F .		Vacue / Phase Fraction	0,0000
Coolant	CoolingDuty	4.520e+006	Btu/hr	Conditions	Temperature IF}	140.0
Glycol	GlycolProduction	713.4	barrel/day	Properties	Pressure (psia)	16.16
					Molar Flow (brole/hr)	618.5
Marci DataBash	1 1 1	1	an e feitig	CONFORMALL	Mats Flow (b/hr)	1971
Alew Traregook	<b>.</b>			K Value	Std Ideal Liq Vol Flow [USGPM]	38.74
				User Variables	Molar Enthalpy (Blu/Ibmole)	-1.409e+00
					Molar Entropy (Btu/Ibmole-F)	3.845
				NOCES	Heat Flow (Btu/te)	-8.7137 <del>e+</del> 0
				Cost Parameters	Lig Vol Flow @Std Cond [barrel/day]	1415.
					Fkad Package	Basis-1
					A construction of the construction of the construction of the function of the construction of the construc	n waa commension, nin ko s
				Worksheet	utachmenis Dynamics	

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

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

Object	Variable	Value	Units	W. Martin and San	Shear Name	Reactor Pro
Reactor	ReactorTemp	190.0	F	WURLINGA	Vacour / Phase Fraction	0,000
Coolant	CoolingDuty	4.111e+006	Blu/hr	Conditions	Termerature IFI	180
Glycol	GlycolProduction	745.5	barrel/day	Procerbes	Pressure Insial	16.1
					Moler Flow Bomole/tv)	612
	4	1 - 1 - 1 - 1 - 1 - 1 - 1 - 1 - 1 - 1 -		Lomposition	Mass Flow (b/hr)	197
View <u>U</u> ałaBook			•	K Value	Std Ideal Lig Vol Flow [USGPM]	38.5
analysis and the second s		1999 - AR - 11 (1990 - 1987 - 1987 - 1997 - 1987 - 1987 - 1987 - 1987 - 1987 - 1987 - 1987 - 1987 - 1987 - 198		Line: Variables	Molar Enthaloy [Btu/Ibmole]	-1.417e+0
					Molar Entropy (Blu/Ibmole-F)	6.23
				Notes	Heat Flow (Btu/hr)	-8.6728e+
				Cost Parameters	Liq Vel Flow @Std Cond (barrel/day)	1414
					Fluid Package	Basis-1
				The Second		·····································
						J
						, 15 
					technents Dynamics	, K

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

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

State	Base Case	180F React			1	
Reactor Temp [F]	140.0	190.0		l	[	1
Cooling Duty [Blu/hr]	4.520e+00E	4.111e+00E				
<b>Glycol Production (ba</b>	713.4	745.5				
	-					
	BB:00000000000000000000000000000000000		11 TO 40 BALOD - (17-1) 113 114 PA	Lancester (14/11-140002-19-04)	 	
						4 m
						-
	n 191-1,					· · · · · · · · · · · · · · · · · · ·
	- 10a		in and the second second	l Barto Maine Angle	1 	1

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

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

### Further Study

For other chemical case examples, see the Applications section. Applications beginning with "C" explore some of the types of chemical simulations that can be built using HYSYS. See **Chapter 5 - Reactions** in the Simulation Basis manual for more information.

## 5.2.5 Reactions Tab

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

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

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

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

The Reaction tab appears as shown in the following figure.

Rich Components	Reactions	Martin Martin	Acaction Sets	5 x - 5 x - 77
H20	- Ban-1	View Ryn	Global Rxn Set	View Set.
12-C3diol		Add Binn		Add Set
Nitrogen	in an	Delete Fixn		Delete Set
		Copy Rag		Copy Set
1. S.	a line and a second sec		Assoc Fluid Pkgs	Import Set
				Export Set
a jami Alana Alana alana				Add to FP
Add Longs.		and the second se	The second second second	. All and a second of the seco

Use the Reaction Manager to do the following:

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

## Adding a Reaction

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

### **Editing a Reaction**

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

## **Deleting a Reaction**

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

## **Copying a Reaction**

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

Figure 5.9
Copy Reactions 🔀
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n personal and a second se
New Reaction Type
C Smple Rate
C Equilitation
C Heterogeneous Cetalytic
Lopy Heaction

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

## Adding a Reaction Set

- 1. Click the Add Set button. The Reaction Set view appears.
- 2. In the Active List column, click the <empty> cell and use the dropdown list to select the reaction you want to add to the set.
- 3. In the Inactive List column, click the <empty> cell and use the dropdown list to select the reaction you want to add to the set. This reaction remains inactive, but it is included in the set.
- 4. From the Solver Method drop-down list, select the reaction solver method you want to use.
- 5. Add any of the available reactions to the set (as long as they are the same type). A single reaction can be added to as many sets as necessary.

Available reaction solver methods:

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

## **Editing a Reaction Set**

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

## **Deleting a Reaction Set**

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

## **Copying a Reaction Set**

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

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

## Importing a Reaction Set

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

## **Exporting a Reaction Set**

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

## Adding a Reaction Set to a Fluid Package

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

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

## 5.2.6 Component Maps Tab

See Chapter 6 - Component Maps in the Simulation Basis manual for additional information. The Component Maps tab allows you to map fluid component composition across fluid package boundaries. Composition values for individual components from one fluid package can be mapped to a different component in an alternate fluid package. This is useful when dealing with hypothetical oil components.

Comp	shent Mapping ping components tr	om Basis-1	<u> </u>	to Bas	is-1	T Clev	ite Collection
Collec	liona			<u></u>	Maps for Colle	iction	
	From Basis	To Basis	Collection		Collection	Coll 1	•
	Bass-1	Basis-1	Loli 1 Fall 2			<i>n</i> , 1	
¥.,	Basis-5	Basis-1	Coll 3	······································	I merely		Add
						8	<del>اروب زیر پر پر پر کرد.</del> ان ک
						1995 - 1 1995 - 1	More .
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Two previously defined fluid packages are required to perform a component mapping. One fluid package becomes the target component set and the other becomes the source component set. Mapping is performed using a matrix of source and target components. The transfer basis can be performed on a mole, mass or liquid volume basis.

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

# 5.3 Reactions

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

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

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

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

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

#### Reactions

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

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

# 5.3.1 Manipulating Reactions

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

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

## 5.3.2 Conversion Reaction

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

Consider the following Conversion reaction:

$$A + \frac{b}{a}B \to \frac{c}{a}C + \frac{d}{a}D \tag{5.1}$$

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

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

\_

5-9

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

$$N_{A} = N_{A_{o}}(1 - X_{A})$$

$$N_{B} = N_{B_{o}} - \frac{b}{a}N_{A_{o}}X_{A}$$

$$N_{C} = N_{C_{o}} + \frac{c}{a}(N_{A_{o}}X_{A})$$

$$N_{D} = N_{D_{o}} + \frac{d}{a}(N_{A_{o}}X_{A})$$
(5.2)

where:  $N_* =$  The final moles of component \* (\*= A, B, C and D)  $N_{*o} =$  The initial moles of component \*  $X_A =$  The conversion of the base component A

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

## Stoichiometry Tab

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

· Section		Ta S	Lind.
Statchiogetry into	1 Mola Wainty	Stoich Coeff	
Methane	16.043	1.000	137
H20	18.015	-1.000	+
00	28.011	1.000	-
Hydrogen	2.016	3.000	1
**Add Comp**			ļ
	Balance Ence	0.00000	1 <u>8</u> .
Balance	Reaction Heat (25.C)	2.1e+05 kJ/kgmole	
Chainking and			

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

#### Reactions

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

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

Basis Tab

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

	Tana and	in the state of the	
Base Co		Methane	
Rim Pha	10 · · · · · · · · · · · · · · · · · · ·	VapourPhase	
CI		40.00 <emply></emply>	
C2	and the second s	<empty></empty>	[16] 동안
Conversio	n (%) = Co + C1*T + C2*1	2	
(T in Kelvi	n)-		
Sim			7 <b>*</b> 11.4

The Reaction Heat value is calculated and displayed

below the Balance Error. A positive value indicates that the reaction is endothermic.

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

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

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

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

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



**Conversion Reactor icon** 

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

## 9.2.2 Conversion Reactor Reactions Tab

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

The Reactions tab, consists of two pages:

- Details
- Results.

## **Details Page**

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

Reactions	Conversion Reaction Details			-
Detail:	Reaction Set Combustor F	Ixn Set 💌 Beaction	n Rixn-1	2
Results	@ Stoichiometay C Basis	Conversion X	Yiew Reaction.	
	Staichiometry Info			
	Component	Mole Wgt.	Stoich Coeff	
	Methane	16.043	-1.000	
	H20	18.015	-1.000	
		28.011	1.000	
	Hydrogen	2.016	3.000	
	"Add Lomp"	v .		t .
				2
	Ba	ance Ellor	0.00000	
	ine ine	scoon meat (20 L)	2. Te+up KJ/Kgmole	
	-			

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

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

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

### Stoichiometry Radio Button

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

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

Component	Mole Wgt.	Stoich Coeff
Methane	16.043	-1.000
H20	18.015	-1.000
C0	28.011	1,000
Hydrogen "Add Comp"	2.016	3.000

#### Basis Radio Button

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

asis Base Component Mether Rim Phase VapourPhe: Co	Component Methane
Base Component Mether Tim Phase VapourPhase	Component Methane
Rin Phase VapourPhas	
o	Phase VapourPhase
N	40
	<emp< td=""></emp<>
2 <er< td=""><td><errc< td=""></errc<></td></er<>	<errc< td=""></errc<>
conversion (%) = Co + C1*T +C2*T^2	ereion (%) = Co + C1*T +C2*T^2

#### **Conversion Radio Button**

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



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

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

Reactors

#### **View Reaction Button**

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

ichiometry Info	-	
Component	Mole Weight	Stoich Coeff
Methan	16.043	-1.000
H20	18.015	-1.000
CC	28.011	1,000
Hydroge "Add Comp"	2.016	3.000
Bglance	Balance Enor Reaction Heat (25 C)	0.00000 2.1e+05 kJ/kgmole

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

## **Results Page**

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

- Reaction Extents
- Reaction Balance.

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

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

#### **Reaction Extents Radio Button**

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

<ul> <li>Descoon</li> </ul>	CREAK		G. Parating Fridayla					
		( risecu	on balance					
	Rank	Act %Cnv	Base Comp	Rxn Extent				
Pixm-1	11	18.09	Methane	4.923				
Rian-2		33.60	Methane	9.144				
Fixer-3	0	48.31	Methane	13.15				
		And a second second						
	-							

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

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

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

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

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

#### **Reaction Balance Radio Button**

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

Reaction Bala	ance	
Total Inflow	Total Rxn	Total Outflow
27.22	-27.22	0.0000
274.8	3.089	277.9
36.29	4.923	41.21
27.22	22.29	49.51
217.7	51.34	269.1
96.93	1.249e-014	98.93
26.30	-26.30	0.0000
· · · · · · · · · · · · · · · · · · ·		
	and the second	
	(* Reaction Bak Total Inflow 27.22 274.8 36.25 27.22 217.7 98.93 26.30	Image: Weight of the section balance           Total Inflow         Total Rim           27.22         -27.22           274.8         30.995           36.29         4.923           27.22         2.23           217.7         51.34           98.93         1.249e-014           26.30         -26.30

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

# 9.2.3 CSTR Reactions Tab

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

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



CSTR icon