In this session you will learn how to install a conversion reactor in HYSYS 3.0.

The references for this section are taken from the 2 HYSYS manuals: Simulation Basis: Chapter 5 Reactions Operations Guide: Chapter 9 Reactors

Reactors.

Taken from: Steady-State Modeling 9.1 The Reactor Operation

With the exception of the PLUG FLOW REACTOR (PFR), all of the reactor operations share the same basic property view. The primary differences are the functions of the reaction type (conversion, kinetic, equilibrium, heterogeneous catalytic or simple rate) associated with each reactor. As opposed to a SEPARATOR or GENERAL REACTOR with an attached reaction set, specific reactor operations may only support one particular reaction type. For instance, a CONVERSION REACTOR will only function properly with conversion reactions attached. If you try to attach an equilibrium or a kinetic reaction to a CONVERSION REACTOR, an error message will appear. The GIBBS REACTOR is unique in that it can function with or without a reaction set.

Thought to remember: CONVERSION REACTORS must have a CONVERSION REACTION SET.

The remainder of this chapter discusses the features of each of these reactors: Sections 9.2-9.4 **GIBBS REACTOR, EQUILIBRIUM REACTOR, CONVERSION REACTOR** or (General Reactors) and **CSTR**.

Reaction Sets (portions from Simulation Basis: Chapter 5 Reactions)

Reactions within HYSYS are defined inside the Reaction Manager. The Reaction Manager, which is located on the Reactions tab of the Simulation Basis Manager, provides a location from which you can define an unlimited number of Reactions and attach combinations of these Reactions in Reaction Sets. The Reaction Sets are then attached to Unit Operations in the Flowsheet.

HYSYS Conversion Reactors – Tutorial on Styrene

Styrene is a monomer used in the production of many plastics. It has the fourth highest production rate behind the monmers of ethylene, vinyl chloride and propylene. Styrene is made from the dehydrogenation of ethylbenzene:

$$C_6H_5-C_2H_5 \Leftrightarrow C_6H_5-CH = CH_2 + H_2$$
(1)

🔊 NoName.hsc - HYSYS 3.0.1 File Edit Basis Tools Window Help **1** 6 2 🖬 📗 Start a New Case

Procedure to Install a Conversion Reaction Set:

- 1. Start HYSYS
- 2. Open a new case by clicking on the blank white page OR use the commands *File New*.
- 3. Since these compounds are hydrocarbons, use the Peng-Robinson thermodynamic package.

NoName_2.hsc - HYSYS 3.0.1

- (Additional information on HYSYS thermodynamics packages can be found in the Simulation Basis Manual Appendix A: Property Methods and Calculations. Note an alternative package for this system is the PRSV)
 - 3.1. Select the Fluid Pkgs menu tab and Press the Add button
 - 3.2. Select the EOS filter radio button to see only Equations of State (EOS)
 - 3.3. Then select the Peng Robinson Equation of State.
 - 3.4. Notice that you have a choice calculating the enthalpies. You

can either use the equation of s can use a prediction method ca

Pitzer method. For this tutorial we will use the equation of state method.

3.5. Press the View button to start adding chemical compounds

n in u state – This will be discussed in alled the Lee-Kesler Method wh	Enter Sigulation Environment.
Simulation Basis Manager Current Fluid Packages	Flowsheet - Fluid Pkg Associations Flowsheet - Fluid Pkg Association EOS Enthalpy Method Specification EQU Enthalpy Method Specification Flowsheet - Fluid Pkg Association Peng Robinson Options HYSYS Standard HYSYS Standard
Sour PR Sour SRK SRK Zudkevitch Joffee	□ Use EOS Density □ Smooth Liquid Densy □ Smooth Liquid Densy
Component List Selection Component List - 1 Set Up Parameters Binary Coeffs StabTest Phase Delete Name Basis-1 Property Pkg	View Corder Roms Tabular Notes Peng Robinson Edit Properties



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4. Install the chemicals for a styrene reactor: ethylbenzene, styrene, and hydrogen. If they are not in the order given below then use the Sort List... button feature.



6. Now return to the Simulation Basis Manager by closing the Component List View window.

Press the <i>Close</i> button or X	
7. Select the Rxns tab	
and then press the 📕 🔓 Fluid Package: Basis-1	
Simulation Basis	
Mgr button.	Press here to
8. The Reaction	start adding
Component Selection	Reaction TXNS
view will appear.	nn Basis Mor
9. Press the Add Rxn	
button	
10. To install a reaction,	
press the Add Rxn	
button.	Edit Properties
Simulation Basis Manager	
Rxn Components Reactions Reactions	
E-Benzene View Rxn Global Rxn Set	
Hydrogen	Add Set
Add Delete Rxn	Delete Set
Reaction Copy Rom	Cop <u>v</u> Set
	Import Set
	Export Set
Add Comps	Add to FP
Components Fluid Pkgs Hypotheticals Oil Manager Reactions Component Mans UserPr	roperty

11. Then select the Conversion Reaction *Refer to Section 4.4 of the Simulation Basis Manual for information concerning reaction types and the addition of reactions.*

12.

🕴 Reacti 💶 🗙	Conversion Reaction: Rxn-1
Conversion Equilibrium Heterogeneous Catalytic Kinetic Simple Rate	Component Mole Weight Stoich Coeff ***Add Comp** -
Add <u>R</u> eaction	Stoichiometry Basis Delete Name Not Ready

On the Stoichiometry tab add all of the components to the component list by using the drop down list.

Select **ethylbenzene** from the drop down list in the Edit Bar. The Mole Weight column should automatically provide the molar weight of ethylbenzene. In the Stoich Coeff field enter a stoichiometric coefficient of -1 (i.e. 1 moles of ethylbenzene will be consumed). Notice that the coefficient will be negative for reactants and positive for products.

- 13. Notice that the units of the Reaction Heat or the Heat of reaction are SI. If you do not have this go to Tools Preferences and load the styrene.prf that you saved from the previous tutorial.
- 14. Now define the rest of the Stoichiometry tab as shown in the adjacent figure. Go to Basis tab and set ethylbenzene as the Base Component and Conversion to 80%. The status bar at the bottom of the property view should now show the Ready message. Note that the conversion reaction can be a function of temperature. This is a simple polynomial fit to conversion as a function of temperature data. Using this type of reaction set we will

🕙 Conversion Reaction: R	xn-1	X
		
Stoichiometry Info		
Component	Mole Weight	Stoich Coeff
E-Benzene	106.166	-1.000
Styrene	104.152	1.000
Hydrogen	2.016	1.000
Add Comp		
Palanaa	Balance Error	0.00000
	Reaction Heat (25 C)	1.2e+05 kJ/kgmole
Stoichiometry Basis		
Delete <u>N</u> ame	Rxn-1	Not Ready

🕙 Conversion Reaction: Rxi	n-1
Basis	
Base Component	E-Benzene
Rxn Phase	Overall
Co	80.00
C1	<empty></empty>
C2	<empty></empty>
Conversion (%) = Co + C1*T +	C2×T^2
(Tin Kelvin)	
Delete <u>N</u> ame	Rxn-1 Ready

be able examine mole and energy balances without knowing the chemical kinetics.

- 15. Close the property view.
- 16. By default, the Global Rxn Set is present within the Reaction Sets group when you first display the Reaction Manager. However, for this procedure, a new Reaction Set will be created. Press the Add Set button. HYSYS provides the name Set-1 and opens the Reaction Set property view.
- 17. To attach the newly created Reaction to the Reaction Set, place the cursor in the <empty> cell under Active List.

Simulation Bas	is Manager	Add Set B	utton	
Pxn Components E-Benzene Styrene Hydrogen	Reactions Exn-1	View Rgn Add <u>B</u> xn Delete Rxn Capy Rx <u>n</u>	Assoc. Fluid Pkgs	View Set Add Set Delete Set Copy Set Import Set
Add Comgs	Hypotheticals Oil Mar	ager Reactions Co	omponent Maps UserProp	Add to FP

18. Open the drop down list in the Edit Bar and select the name of the Reaction.

Rxn-1 The

Set Type will correspond to the type of Reaction which you have added to the Reaction Set. The status message will now display Ready. (*Refer to Section 5.4 – Reaction Sets for details concerning Reactions Sets.*)

- 19. Press the Close button to return to the Reaction Manager.
- 20. To attach the reaction set to the Fluid Package (your peng robinson thermodynamics), highlight Set-1 in the Reaction Sets group and press the Add to FP button. When a Reaction Set is attached to a Fluid Package, it becomes available to unit operations within the Flowsheet using that particular Fluid Package.
- 21. The Add 'Set-1' view appears, from

which you highlight a Fluid Package and press the Add Set to Fluid Package button.

- 22. Press the Close button. Notice that the name of the Fluid Package (Basis-1) appears in the Assoc. Fluid Pkgs group when the Reaction Set is highlighted in the Reaction Sets group.
- 23. Now Enter the Simulation Environment by pressing the button in the lower right



Freaction S	et: Se	et-1			
Name Set-1					
Set Info					
Set Type		Conversion	Ready	/	<u>A</u> dvanced
			Independ	lent	<u>R</u> anking
Active List	OK	Inactive	List	Opera	tions Attached
Rxn-1 <		∫ <er< td=""><td>mpty></td><td></td><td></td></er<>	mpty>		
View Active		View Inc	active	ļ	
Make Inactive -≥		<u>≺</u> - Make	Active		





- 24. Install a conversion reactor. Either through the
 - 24.1. Flowsheet, Add operation
 - 24.2. f12
 - 24.3. or icon pad. Click on General Reactors and then a small pad pops up with a choice of 3 reactors. Choose the conversion reactor. Click on the Conversion Reactor icon, then release left mouse button. Move cursor to pfd screen and press left mouse button. Double click on the reactor to open.
- 25. Add stream names and a new reactor name as shown. After naming these streams the following errors appear: Requires a Reaction Set and Unknown Duty.



e i CUSTOM FLOW 🖞 UnitOps - Case (Mair - × Available Unit Operations Cont. Stirred Tank Reactor C All <u>U</u>nit Ops Conversion Reactor Equilibrium Reactor Gibbs Reactor Plug Flow Reactor Cancel Heat Transfer Equipr Rotating Equipme Piping Equipment Solids Handling Reactors Prebuilt Columns Short Cut Colum Sub-Flowsheets Logicals Extension: User Ops

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Case (Main)

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General Reactors

- 26. Next add the reaction set by selecting the reactions tab and choosing Reaction Set from the drop down menu.
- 27. Close the Conversion Reactor
- 28. Open the workbook



- 29. Now add a feed composition of pure ethylbenzene at 217 gmol/s, 880 K, 1.378 bar. Remember you can type the variable press the space bar and type or select the units.
- rersion Reactor Set-1 _ 🗆 × Con Conversion Reaction Details Reactions Set-1 Details Reactio<u>n</u> Set -Reaction Byn-1 -Results Stoichiometry 🔿 Basi Conversion % ⊻iew Reaction... etrv Info 106.166 104.152 2.016 1.000 1.000 1.000 E-Benzen Styren Hydrogen **Add Comp** Balance Error Reaction Heat (25 C) 0.00000 1.2e+05 kJ/kgmole Design Reactions Rating Worksheet Dynamics Delete ☐ Ignored
- 30. Isn't it strange that you can't see the molar flowrate

in the composition window? Let's add the molar flowrates to the workbook windows. Go to *Workbook Setup* using the menu commands at the top of your screen.

31. Press the Add button on the right side32. Select Component Molar Flow and then press the All radio button.

🎽 Setup		×	1
Workbook Tabs Material Streams Add Compositions Energy Streams Unit Ops	o Contents bject Name: Compositions Type: Material Stream ariables Variable Forma Comp Mole Frac (E-Be 1.4 fix Comp Mole Frac (Styre 1.4 fix Comp Mole Frac (Hydr 1.4 fix	at <u>U</u> se Set ec <u>Add</u> ec <u>Delete</u> <u>Ec Format</u>	Add Button
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- 38. Now run the simulation. For an isothermal reactor specify the outlet temperature.
- 39. For the adaiabatic reactor, **delete** the temperature specification and specify the heat duty as 0. The heat duty can be specified in several ways:
 - 39.1. in the workbook under the Energy Streams tab
 - 39.2. in the reactor in the Design Tab under the parameters option in Duty.

💐 styrene conversion reactor.hsc - HY5Y5	
Eile Edit Simulation Flowsheet Tools Window Help	
🗅 🖆 🖬 🕂 🕮 🛤 🎼 💳 🏷 🐨 🐨 🌡 🖗	Environment: Case (Main) Mode: Steady State
N Conversion Deactor - Set-1	Workhook - Case (Main)
Design IF Act as a Separator When Cannot Solve Connections Single Phase Vessel Volume User Variables Delta P 0.0000 kPa Liquid Level 50.00 % Duly Liquid Volume Heating Cooling Design Reactions Rating Wotksheet Delete Unknown Duty Duty Ignored	Name Reactor Head D ** New ** Head Flow [kJ/s] (empty) (empty
	Unknown Duty warning
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40. Now change the conversion. The changes that we will make now will only effect this reactor. Go to the reactions tab in the reactor. Select the Conversion% radio button. Now type a new conversion value. Notice that this is in percent conversion. Use the spread sheet operations to check you conversion values.



At the end of this exercise submit a printout with the following:

- 1) Make the following plots from your Conversion reactor simulation:
 - a) The effect of conversion of ethylbenzene on the heat duty of an isothermal reactor at a constant temperature of 250°C.
 - b) The effect of inlet temperature on outlet temperature for an adiabatic reactor at a conversion of ethylbenzene of 80%.
- 2) Printout the following from **one** simulation on HYSYS

Reactor Summary:

Double click on reactor Undo push pin if present Select Print from main menu Then select the Datablock(s) shown in the second figure:

Property Package

Simulation, Enter Basis Environment Select View Print Select Preview... Then print the one page document

Reactions

Go to Rxns tab of the fluid package view Double click on your reaction Undo push pin Select Print Preview And printout this one page view

Process Flow Diagram Click on pfd and choose print

Workbook Select workbook and print.

Reactions Equilibrium Reaction Details Details Regation Set: HYSYSequilibrium Reaction: Results Stoichiometry © Basis © Keq © Approcent to the Wgt Stoichiometry Igfo Stoichiometry Igfo Stoichiometry Igfo Hydrogen 2016 Hydrogen 2016 Hydrogen 2016 Design Balance Error Design Select All Northsheet Invert Selection Dynemics Set Preferences Use Preferences Use Preferences keed Datablocks will be included in the Datasheet. blocks with trailing ellipses have additional options that ppear here when selected. Select Datablocks Select All	
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