In this session you will learn how to install a tubular reactor in HYSYS with a kinetic reaction rate. This HYSYS reaction rate will allow specification of an irreversible reaction. We will ignore equilibrium in this tutorial.

The references for this section are taken from the 2 HYSYS manuals: Simulation Basis: Chapter 4 Reactions Steady-State Modeling: Chapter 9 Reactors

## **Reactors.**

Taken from: 9.7 Plug Flow Reactor (PFR) Property View

The PFR (Plug Flow Reactor, or Tubular Reactor) generally consists of a bank of cylindrical pipes or tubes. The flow field is modeled as plug flow, implying that the stream is radially isotropic (without mass or energy gradients). This also implies that axial mixing is negligible.

As the reactants flow the length of the reactor, they are continually consumed, hence, there will be an axial variation in concentration. Since reaction rate is a function of concentration, the reaction rate will also vary axially (except for zero-order reactions).

To obtain the solution for the PFR (axial profiles of compositions, temperature, etc.), the reactor is divided into several subvolumes. Within each subvolume, the reaction rate is considered to be spatially uniform.

You may add a Reaction Set to the PFR on the Reactions tab. *Note that only Kinetic, Heterogeneous Catalytic and Simple Rate reactions are allowed in the PFR.* 

Reaction Sets (portions from Simulation Basis: Chapter 4 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 PFR Reactors using kinetic rates- Tutorial using Styrene

Styrene is a monomer used in the production of many plastics. It has the fourth highest production rate behind the monomers 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)

In this reactor we will neglect the aspect that reaction 1 is an equilibrium reaction and model this system using a power law expression. In HYSYS this is called a *Kinetic Rate* expression. The reaction rate expression that you will install is given by the following:

$$r_{EB} = -4.24 \times 10^{3} \frac{\text{mol EB}}{\text{L}_{\text{reactor}} \text{kPa s}} p_{EB} \exp \left[ -\frac{21708 \text{ cal/mol}}{\left(1.987 \frac{\text{cal}}{\text{mol K}}\right)T} \right]$$
(2)

Notice that the reaction rate has units and that the concentration term is partial pressure with units of kPa.

### **Procedure to Install a Kinetic Reaction Rate:**

1. Start HYSYS

A Fluid Pack

-Current Reaction S

Associated Reacti

Prop Pkg / Corr

Delete

Rxn Components

Add Comps.

2. Since these compounds are hydrocarbons, use the Peng-Robinson thermodynamic package. (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)

Fluid Package: Ba	asis-1		×
Current Component E-Benzene Styrene Hydrogen	List Add Comps Add Comps C Libray C Hypothetical C	Components Available From The Pure Component Library Match ethylb Use Filter Family Filter C SimName © FullName / Synonym © Formula ETBE Ethyltert-Bulylether C6H140 BromoC2 Ethyltermede C2H58r 12BromoC2 Ethylene Bromide C2H58r 12BromoC2 Ethylene Bromide C2H4Br2 Ethynyl-BZ Ethyrnyl-BZ C8H6 Ethynyl-BZ EthynylBenzene C8H6	
Prop Pkg Com Delete	Sort List ponents Parameters Name Basis-1	Image: Show Synonyms         Image: Cluster           Binary Coeffs         StabTest         Phase Order         Rxms         Tabular         Notes           Property Pkg         Peng Robinson	

- 3. Install the chemicals for a styrene reactor: ethylbenzene, styrene, and hydrogen. If they are not on this list then use the Sort List... button feature.
- 4. Now return to the Simulation Basis Manager by either closing the Fluid Package Basis-1 window or clicking on the Rxns tab and pressing the Simulation Basis Mgr... button.



add components

5. On the Reactions tab of the Simulation Basis Manager, press the Add Comps button.

- 6. The Reaction Component Selection view will appear. In the Add Comps group, ensure that the FPkg Pool radio button is selected. This will make only the Fluid Package components available to the Reaction Manager.
- 7. Highlight the Fluid Package in the Available Fluid Pkgs group.
- 8. Press the *Add This Group of Components* button to transfer the fluid package components into the Selected Reaction Components group.
- Press the *Close* button ⊠ to return to the Reactions tab. The selected components are present in the Rxn Components group.
- 10. To install a reaction, press the Add Rxn button.
- 11. From the Reactions view, highlight the Kinetic reaction type and press the Add Reaction button. The property view for the Reaction is opened. *Refer to Section 4.4 of the Simulation Basis Manual for information concerning reaction types and the addition of reactions.*
- 12. On the Stoichiometry tab select the first row of the Component column in Stoichiometry Info matrix. 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 -1 (i.e. 1 moles of ethylbenzene will be consumed).

- 13. Now define the rest of the Stoichiometry tab as shown in the adjacent figure. Go to Basis tab and set the Basis as partial pressure, the base component as ethylbenzene and have the reaction take place only in the vapor phase. The pressure basis units should be kPa and the units of the reaction rate were given above as mol/(L s). Since the status bar at the bottom of the property view shows Not Ready, then go to the Parameters tab.
- 14. Add the pre-exponential no units and the activation energy with units of cal/mol (which is transformed to kJ/kmol after entry.) Leave  $\beta$  blank or place a zero in the cell. Notice that you don't enter the negative sign with the pre-exponential.

🗏 Kinetic Reaction: Rxn-1 🛛 🔜 🗙	🎽 Kinetic Reaction: Rxn-1 🛛 🛛 💌 💌
Basis       Partial Pres         Basis       Partial Pres         Base Component       E-Benzene         Rxn Phase       VapourPhase         Min. Temperature       0.0000 K         Max Temperature       3273 K         Basis Units       IXPa         Bate Units       gmole/L-s	Equation HelpA4.2e+03E9.1e+04B <empty>C<empty>Reverse ReactionA'<empty>B'<empty>B'<empty></empty></empty></empty></empty></empty>
Stoichiometry Basis Parameters	Stoichiometry Basis Parameters
Delete Name Rxn-1 Not Ready	Delete Name Rxn-1 Ready

#### 🎽 Kinetic Reaction: Rxn-1 Stoichiometry and Rate Info Component Mole Wt. Stoich Coeff Fwd Order Rev Order 106.166 E-Benzene 1.000 104.152 Styrene 1.000 2.016 0.00 Hydrogen 1.00 \*Add Comp\* Balance Error 0.00000 Balance Reaction Heat (25 C) 1.2e+05 kJ/kgmole Stoichiometry Basis / Parameters Delete Name Rxn-1



Reactions

Heterogeneous Catalytic

Add <u>Reaction</u>

Conversion Equilibrium

Kinetic Simple Rate

ted with the Fluid Pa

Available Fluid Pkgs

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ated Com

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- 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.
- 18. Open the drop down list in the Edit Bar and select the name of the Reaction. The Set Type will correspond to the type of Reaction that you have added to the Reaction Set. The status message will now display Ready. (*Refer to Section 4.5 – 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 hand portion







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Plug Flov

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FLOW DUSTOM SHEET DOLUMIN

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- 24. Install a PFR reactor. Either through the
  - 24.1. Flowsheet, Add operation
  - 24.2. f12
  - 24.3. or icon pad. Click on PFR, 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 as shown. After naming these streams the following errors appear: Requires a Reaction Set and Unknown dimensions.
- 26. Next add the reaction set by selecting the reactions tab and choosing Reaction Set from the drop down menu.
- 27. Go to the Ratings Tab. Remember in the case of distillation columns, in which you had to specify the number of stages? Similarly with PFR's you have t

specify the volume. In this case add the volume as  $0.77 \text{ m}^3$  and length 3 m as shown in the figure.

- 28. Return to the Design tab and specify that this reactor has no pressure drop and is an adiabatic reactor.
- 29. Close the PFR Reactor



- 31. Now add a feed composition of pure ethylbenzene at 152.2 gmol/s, 880 K, 1.378 bar. Remember you can type the variable press the space bar and type or select the units.
- 32. 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.
- 33. Press the Add button on the right side
- 34. Select Component Molar Flow and then press the All radio button.

🎽 Setup		×
Workbook Tabs          Material Streams       Add         Compositions       Delete         Unit Ops       Delete	Tab Contents         Object       Order.         Name:       Compositions       Order.         Type:       Material Stream       New Type         Variables       Variable       Format       Use Se         Comp Mole Frac (E-Be       1.4 fixec       Add.         Comp Mole Frac (Styre       1.4 fixec       Delet         Eormat       Eormat       Order.	Give it a new name such as Compositions
Select Variable(s) ForMain	×	
Variable     Variable Specs       Steady State Specs     ▲       Vapour Fraction     ▲       Temperature     ▲       Pressure     ▲       Molar Flow     ▲       Liquid Volume Flow     ▲       Heat Flow     ■       Power     Std Liq Vol Flow Spec       Comp Mole Frac     ▲       Comp Moler Flow     ✓       Comp Molar Flow     ✓       Description     Comp Molar Flow	All/Single Single Single All/Single Single Single Comp Molar Flow <u>Cancel</u> <u>Comp</u> <u>Molar</u> Comp	ene.PRF)
35. To change the units of the	a variables go to Tools	

 To change the units of the variables go to Tools, preferences

Load Preference Set.

Simulation Variables Reports Files Resources Extensions Oil Input / Tray Sizing

Save Preference Set..

- 36. Then either bring in a previously named preference set or go to the variables tab and clone the SI set and give this new set a name.
- 37. Change the component molar flowrate units from kmol/hr to gmol/s.
- 38. Change the Flow units from kmol/hr to gmol/s
- 39. Next change the Energy from kJ/hr to kJ/s.
- 40. Save preference set as well as the case. Remember that you need to open this preference set every time you use this case.
- 41. Notice that the reactor has converged after you added the conditions of the feed stream.
- 42. To run an isothermal reactor you need to delete the duty that was specified (in blue) and specify the outlet temperature. Try it! Isn't that easy!
- 43. Examine the output in the reactor screens by opening the reactor. Go to the Performance tab and make a plot of the composition profile. Notice that you will have to bring the compositions into the plot.

## **POLYMATH and Hand Calculations**

44. Now we will look at verifying what is going on in HYSYS. Notice that HYSYS is a black box calculation. You can't see what it is doing. Reading the help files will give an indication on how it is integrating the reactor. To fully understand the PFR let's go to some hand calculations given on the following page.

Styrene Example - Simple Rate 1/2

Polymath Setup  
T=880K  

$$r_{E6} = -k P_{EB}$$
  
 $k = 4.24 \times 10^{3} \frac{M0!}{5L kla} \exp\left[-\frac{21708 (al/mol)}{1.987 cal}\right]$   
 $k = 0.017206 \frac{M0!}{5L kla} \exp\left[-\frac{21708 (al/mol)}{1.987 cal}\right]$   
 $k = 0.017206 \frac{M0!}{5L kla}$   
 $\frac{M0DEL}{M0DEL}$   
 $\frac{M0DEL}{dV} = V_{EB}$   
 $\frac{M0DEL}{dV} = V_{EB}$   
 $\frac{M0DEL}{dV} = V_{EB}$   
 $\frac{M0DEL}{dV} = V_{EB}$   
 $\frac{1}{52.2} \frac{1}{52.2} \frac{1}{5$ 

 $\sim$ 

Styren Simple Rate 2/2  $\frac{dF_{EB}}{dV} = \frac{-(F_{EB} - F_{EB_0})}{V} = 2.37 \frac{mol}{Ls}$  3 max rate  $\frac{1}{5} \frac{1}{5} \frac{1}{5} \frac{2.37 \frac{mol}{Ls}}{V} (770L)$  3 max rate  $F_{EB} = \frac{1}{5} \frac{2.37 \frac{mol}{Ls}}{V} (770L)$   $Value & F_{EB}$  = Negative number $s_{0}^{*}$  complete conversion before 770L

# 45. Construct a POLYMATH program to give the following: **POLYMATH Results**

Styrene Kinetic Rate Model 02-20-2002, Rev5.1.230

### **Calculated values of the DEQ variables**

Variable	initial value	minimal value	maximal value	final value
V	0	0	770	770
FEB	152.2	0.2295141	152.2	0.2295141
FS	0	0	151.97049	151.97049
FH	0	0	151.97049	151.97049
FT	152.2	152.2	304.17049	304.17049
P	137.8	137.8	137.8	137.8
Т	880	880	880	880
k	0.0172065	0.0172065	0.0172065	0.0172065
pEB	137.8	0.103978	137.8	0.103978
rEB	-2.3710547	-2.3710547	-0.0017891	-0.0017891

#### **ODE Report (RKF45)**

#### Differential equations as entered by the user

- [1] d(FEB)/d(V) = rEB
- [2] d(FS)/d(V) = -rEB
- [3] d(FH)/d(V) = -rEB

#### Explicit equations as entered by the user

- [1] FT = FEB+FS+FH
- [2] **P = 137.8**
- [3] **T = 880**
- [4] k = 4.24e3\*exp(-21708/1.987/T)
- [5] pEB = FEB/FT\*P
- [6] **rEB = -k\*pEB**

#### Comments

[9] **P = 137.8** *kPa* 

#### Independent variable

- variable name : V
- initial value : 0 final value : 770

#### Precision

Step size guess. h = 0.000001 Truncation error tolerance. eps = 0.000001

#### General

number of differential equations: 3 number of explicit equations: 6 Data file: C:\ACdrive\Courses Jan 2002\Reaction Engineering\Lectures&Examples\styrene\styrene kinetic rate model.pol

46. Now let's compare this solution with that given in HYSYS. Notice that the product flowrates of ethylbenzene from POLYMATH is 0.23 mol/s and from HYSYS is 0.55 mol/s. Why is there a difference?

- 47. Increasing the number of segments used in the integration can reduce the HYSYS product flowrate of ethylbenzene. Go to the following screen and change the number of segments and observe the effect on the product flowrate of ethylbenzene.
- 48. Notice that if you increase the number of segments, then it will take longer to solve this problem. This could be important when using a reactor in a complex chemical plant simulation in you senior year!
- 49. Now examine the following screens:

<sup>388</sup> PFR-100 - S	Set-1	
3.0e-06	m	<b>*</b>
Reactions Overall Details Results	Reaction Info         Reaction Set         Set1         Initialize segment reactions from:         © Cyrrent       © Preyious         Integration Information         Number of Segments         200         Minimum Step Fraction         1.0e-06         Minimum Step Length         3.0e-06 m	
Design Reaction	Rating Worksheet Performance Dynamics	
Delete	OK Igno	ored

				J torkymole						
Reactions Overall Details Results	Reaction Details Reaction: F Specifics: O Basis	lxn-1 Stoichiomet <u>r</u> y	▼ <u>V</u> iew	Reaction	Reactions Overall Details Results	Reaction Balan Reaction Ex Rxn-1	ce Kents C Act. % Cnv. 99.83	Reaction Balan Base Comp E-Benzene	ce Rxn Extent 151.9	
tice all nificant gits are ren	Base Compon A B A' E' B' B'	ent	E-Benz 9.083e- <em <em< td=""><td>2200 1240 1904 1909 1909 1909 1909 1909</td><td></td><td></td><td></td><td></td><td></td><td></td></em<></em 	2200 1240 1904 1909 1909 1909 1909 1909						
	tions Rating World	ksheet / Perform OK	ance (Dynamic	s /		tions Rating (W	/orksheet <u>Perf</u> OK	formance / Dyn	iamics	nored
<b>PFR-100</b> -	Set-1			 gmole/s	▲ PFR-100 - Se	et-1				-# X
PFR-100 -	Set-1			gmole/s	Performance	et-1  • Reaction Rates	g C Compon	ent Production R	lates	-× ×
Peero PFR-100 - 1522 Reactions Overall Details Results	Set-1  Reaction Balance  Reaction Exter  E-Benzene  Styrene  Hydrogen	nts PRe Total In 152 2 0.0000 0.0000	action Balance Total Rxn 151.9 151.9 151.9	Total Out 0.2534 151.9 151.9	PFR-100 - S     Performance     Conditions     Flows     Rxn Rates     Transport     Compositions	€ Fleaction Rates Length [m] 7.500e-03 2.250e-02 3.750e-02 3.750e-02 3.750e-02 9.750e-02 9.750e-02 1.125e-01 1.275e-01 1.425e-01 1.725e-01 1.725e-01 1.725e-01	Rxn-1 [gmole/L-s] 2.131e+00 1.931e+00 1.754e+00 1.621e+00 1.498e+00 1.295e+00 1.295e+00 1.295e+00 1.210e+00 1.134e+00 1.055e+00 1.003e+00 9.468e+01 8.950e+01	ent Production R	iales	
Peerson PFR-100 - 152.2 Reactions Overall Details Results	Set-1  Reaction Balance: C Reaction Exter E-Benzene Styrene Hydrogen	nts PRe Total In 152 2 0.0000 0.0000	action Balance Total Rxn 151.9 151.9 151.9	Total Dut 0.2534 151.9 151.9	PFR-100 - S     Performance     Conditions     Flows     Rxn Rates     Transport     Compositions	€ Fleaction Rates Length [m] 7.500e-03 2.250e-02 3.750e-02 3.750e-02 8.250e-02 9.750e-02 1.125e-01 1.275e-01 1.425e-01 1.725e-01 1.725e-01 1.725e-01	Rxn-1 [gmole/L-s] 2.131e+00 1.754e+00 1.754e+00 1.498e+00 1.295e+00 1.295e+00 1.210e+00 1.134e+00 1.055e+00 1.003e+00 9.468e+01 8.950e+01	ent Production R	Aates	

50. Make a plot of the molar flowrates within the PFR. Go to the Performance tab and click on composition.

At the end of this exercise submit 4 printouts (5 pages total).

- From a word document printout the following (2 pages): (Paste all of your results into one word document.) Make the following plots from your Conversion reactor simulation:
  - a) The effect of inlet temperature on the conversion of ethylbenzene for an adiabatic reactor.
  - b) The effect of reactor temperature on the conversion of ethylbenzene for an isothermal reactor. Hint: you can do this using the Databook. Create a spreadsheet that you can import the feed temperature to a cell B1, then export this temperature from a formula in cell B2 to the product stream. See figures on this page for help.
  - c) POLYMATH program
- 2) On a separate sheet printout the Reaction Summary Printout (See Below for instructions)
- 3) On a separate sheet printout the Reactor Summary Printout

SPRDSHT-1	<u> </u>	SPRDSHT-1
	<b>_</b>	
Current Cell Exported To: Products Exportab	le 🔽	Spreadsheet Name SPRDSHT-1
B2 Variable: Temperature Angles in:	Rad	Cell Object Variable Description Edit Import
A B C 1 Feed Temp 1000 K	<u> </u>	B1 Feed Temperature Add Import
2 Isothermal T 1000 K		Delete Import
4 5		
		Cell Object Variable Description Edit Export
		B2 Products Temperature Add Export
9	• •	Delete Export
Connections Parameters Formulas Spreadsheet Calculation	n Order jøles /	Connections Parameters Formulas Spreadsheet Calculation Order Ales
Delete Function Help Spreadsheet Only		Delete Function Help Spreadsheet Only
SPRDSHT-1	××	SPRDSHT-1
	<u> </u>	
Spreadsheet Parameters Number of Columns 4 Before Pressure-Flow Step		Formula Summary
Number of Rows         10         After Pressure-Flow Step           Units Set         styrene         Each Composition Step		B2 +B1 1000 K
Exportable Cells (Visible in Spreadsheet's Variable List)		
Cell Visible Name Variable Name Variable Typ	ie i	
B2 B2: Temperature Temperature Temperature		
Connections Parameters Formulas Spreadsheet Calculation Order	bles /	Connections Parameters Formulas Spreadsheet Calculation Order des
Delete Function Help Spreadsheet Only	Ignored	Delete Function Help Spreadsheet Only



## **Reaction Summary**

- 1. Go back to the simulation Basis Manager by clicking on the Erlenmeyer flask.
- 2. View the reaction
- 3. Remove the pushpin
- 4. Select File Print and use the preview feature to see the following:
- 5. Print

## **Reactor Summary:**

Double click on reactor Undo pushpin Select Print from main menu Then select the Datablock(s) shown in the Select Datablock(s) to Print for PFR figure:

## Workbook

Select workbook and print.









🎽 Re	eport	Preview - I	Datasheet	t								_ 8 ×
Format/	'Layout	Print Setup	<u>U</u> pdate	<u>P</u> rint	<u>C</u> lose							
	1	0		Rowan I Iniversity		Case Na	ame: C:NAC	drive\Courses	: Jan 2002\F	Reaction Engineering\L	.ectures&Example	
	3	HYPRO	TECH	Calgary, Alberta		Unit Set:	styrer	ne				
	4	LIFEOTOLE	INNOVATION	CANADA		Date/Tin	ne: Wed I	Feb 20 10:50:2	26 2002			
	6 7 8		Plug F	low Read	ctor: PFF	R-100						
	9 10					CONNE	CTIONS					
	11 12					Inlet S	tream					
	13		STREAM N	IAME				FROM UNIT	OPERATION			
	14 15	Feed										
	16					Outlet	Stream					
	17	Draduata	STREAM N	IAME				TO UNIT O	PERATION			
	10	Froducis				<b>F</b>	<b>0</b> 4					
	20		0705444			Energy	stream					
	21	Heat Duty	STREAMIN	AME	Plug Flo	w Reactor		TO UNIT O	PERATION		PFR-100	
	23	Hourbar			1.1.9	PARAM	ETERS					
	24					TANAM						
	26					Physical Pa	arameters					
	27		T	ype : User Specified				Pres	sure Drop:	0.0000 kPa	×	
	28 29				F	leat Transfe	er : Heating					
	30	Т	ype : Direct Q V	/alue	Ene	ergyStream : H	Heat Duty			Duty: 6.791e+00	17 kJ/h	
	31 32					Dimen	sions					
	33	Total Volume:	0.77	700 m3 * Length:		3.000 m *	Diameter:		0.5717 m	Number of Tubes:	1 *	
	34	Wall Thickness:	5.000e	-003 m * Void Fra	ction:	1.0000 *	Void Volume:		0.7700 m3			
	36					Reactio	on info					
	37		Reacti	on Set: Set-1				Initi	alize From:	Current		
	39				li li	ntegration I	Information					
	40	Number of Segme	nts:	:	50 * Minimum Step	p Fraction:		1.0e-06 *	Minimum Step	o Length:	3.0e-06 m	
	41											
<u> </u>	1 + 1	4										Þ

## Report Preview - Datasheet Format/Layout... Print Setup... Update

<u>P</u>rint <u>C</u>lose

1	0			Case Name:	C:\ACdrive\Courses Jan 2002	Reaction Engineerin	g\Lectures&Example		
3	MYPROTECH	Calgary, A	liversity Iberta	Unit Set:	Unit Set: styrene				
1	LIFEOTOLE INNOVATION	CANADA		Date/Time:	Date/Time: Wed Feb 20 10:48:59 2002				
/ / /	Work	book:	Case (Maii	ו)					
0				Material Stream	ıs				
1	Name		Feed	Products					
2	Vapour Fraction		1.0000	1.0000					
3	Temperature	(K)	880.0	* 880.0 *					
4	Pressure	(bar)	1.378	* 1.378					
5	Molar Flow	(gmole/s)	152.2	* 304.1					
3	Mass Flow	(kg/h)	5.817e+004	5.817e+004					
7	Liquid Volume Flow	(m3/h)	66.86	78.58					
з	Heat Flow	(kJ/h)	8.826e+007	1.562e+008					
9				Compositions					
1	Name		Feed	Products					
2	Comp Molar Flow (E-Benze	néamole/s)	152.2000	* 0.3391					
з	Comp Molar Flow (Styrene)	(amole/s)	0.0000	* 151.8628					
4	Comp Molar Flow (Hydroge	n)(qmole/s)	0.0000	* 151.8628					
5				Energy Stream	s				
7	Name		Heat Duty						
3	Heat Flow	(kJ/h)	6.791e+007						
9				Unit Ops					
1	Operation Name	Ope	eration Type	Feeds	Products	Ignored	Calc. Level		
2 3	PFR-100	Plug Flov	/ Reactor	Feed	Products Heat Duty	No	500.0 *		

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