Styrene Reactor

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 form the dehydrogenation of ethylbenzene:

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

This reaction has several undesired side reactions that produce toluene and benzene:

$$C_6H_5 - CH = CH_2 \Leftrightarrow C_6H_5CH_3$$
⁽²⁾

$$C_6H_5 - CH = CH_2 \Leftrightarrow C_6H_6 + CH_2 = CH_2$$
(3)

Now let's look at a simulation of an industrial reactor for styrene production. You will need to get 2 files: a case file and a preference file. Return to <u>http://engineering.rowan.edu/~hesketh/0906-316/index.html</u> and save the files styrene inductive.hsc and styrene.prf. The following link may work: <u>http://engineering.rowan.edu/~hesketh/HYSYS_files/styrene%20inductive.hsc</u> <u>http://engineering.rowan.edu/~hesketh/HYSYS_files/styrene.PRF</u> Next load a preference set called Styrene.prf also found in the same folder. If you would like to read the help manuals for HYSYS they are located at <u>http://engineering.rowan.edu/~hesketh/hysyshelp/Menu.pdf</u>

Open the workbook and do the following:

- 1. Why are there heaters between each reactor. Sketch the temperature, pressure and composition profiles in these reactors.
- 2. What would happen if the heat duty on each of the reactors was set to zero? To do this you must remove heater outlet temperature specifications and set the duty to zero.
- 3. Examine the effect of varying the inlet temperature to the first reactor on the outlet compositions of this process.
- 4. Examine the effect of varying the inlet pressure outlet compositions of this process.

Write and sketch your answers on a separate sheet of paper.

Now let's look at some of the tools in HYSYS

Spreadsheet:

To easily access the variables you may want to use the spreadsheet function within HYSYS.

- Go to the help files and skim the topic in HYSYS 2.4, Steady-State Modeling, Chapter 10 Logical operations, section 10.6 Spreadsheet. See the link to HYSYS help on the Chemical Reaction Engineering Homepage. <u>http://engineering.rowan.edu/~hesketh/0906-316/index.html</u> or go directly to help using http://engineering.rowan.edu/~hesketh/hysyshelp/Menu.pdf
- 2. Open the spreadsheet by using the Flowsheet, Add Operation, click on Logicals radio button and select Spreadsheet.

🚺 UnitOps - Case (Main)		<u></u>
Categories C All <u>Unit</u> Ops C Vessels C Heat Transfer Equipment C Rotating Equipment C Piping Equipment C Solids Handling C Reactors C Prebuilt Columns C Short Cut Columns C Sub-Flowsheets C Logicals C Extensions C User Ops	Available Unit Operations Adjust Balance Digital Pt MPC Controller Parametric Unit Operation PID Controller Recycle Selector Block Set Spreadsheet Stream Cutter Operation Surge Controller Transfer Function Block	<u>A</u> dd <u>C</u> ancel

To easily calculate the conversion of the 3 reactor system install the appropriate variables.

1. Go to the spreadsheet and type in the following names:

SPRDSHT-1				
Current Cell B1 Variable:		Exportable		In your simulation
A 1 EB into system 2 EB leaving system 3 Conversion 4 Feed T 5 6 7 8 9 9	B			you must click on the push pin to remove this button
	s Formulas Spre.	adsheet Calculation O		

2. End by clicking on cell B1

Select Import for cell						
Flowsheet Case (Main) Navigator Scope Flowsheet Case Basis Utility	Object heater1 Heater 2 PFR 1 outlet PFR 2 inlet PFR 2 outlet PFR 3 outlet PFR 3 Outlet PFR Feed Adiabatic PBR 1 Adiabatic PBR 1 Adiabatic PBR 3 Heater 1 Heater 2 FeederBlock_PFR F¢ ProductBlock_PFR 3	Average Liquid Density Comp K Value - Heavy Li Comp K Value - Light Liqu Comp K Value - Mixed Lic Comp Mass Flow Comp Molar Flow Comp Mole Frac Comp Volume Flow Comp Volume Flow Comp Volume Frac Cp/Cv Dynamic P/F Specs Heat Flow Heat Of Vapourization Heavy Liquid Fraction Higher Heating Value	Variable Specifics E-Benzene Styrene Hydrogen H2O Benzene Toluene Ethylene Methane	<u>O</u> K Object Filter ● All ● Streams ● UnitOps ● Logicals ● ColumnOps ● Custom Custom		
Variable Description:	Comp Molar Flow (E-Be	nzenej		<u>C</u> ancel		

3. Using the Edit Import button bring in the following variable:

- 4. Notice that it has placed this in Cell A1. Change this to B1 in the cell edit window.
- 5. Another way to bring in a variable is to drag it into the spreadsheet. (See section 10.6.2). As stated in the help click and hold the right mouse button and drag it over to the spreadsheet in the desired location.
- 6. Next calculate conversion of ethylbenzene in this reactor as shown in Equation 4.

$$\chi_A = \frac{\left(F_{Ao} - F_A\right)}{F_{Ao}} \tag{4}$$

- 7. To see the effect of changing feed temperature on conversion drag the temperature (holding the right mouse button and dragging.)
- 8. Comment on the effect of inlet temperature on conversion.

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1 2 3 4 5 6 7 8 9	A EB into system EB leaving system Conversion Feed T	B 217.5000 gmole/s 45.6586 gmole/s 0.7901 880.0 K					click on the push pin to remove this button to remove it
	Connections / Parame DeleteF	ters Formulas Sp	readsheet	Calculation eet Only	Order Ales		

Open the pdf file for HYSYS help and go to the User's Guide.

Go to the index and find databook. Click on the first entry (it will take you to page 5-15.) Skim through section 5.

Now do the following.

- 1. Add the variables that you had in the spreadsheet:
- 2. Go to the Case Studies Tab
- 3. Add the following case study

A DataBook		× ×
Ayailable Data Entries Object PFR Feed PFR 3 Outlet SPRDSHT-1	Variable Temperature Comp Molar Flow (E-Benzene) Comp Molar Flow (E-Benzene) B3:	Edit Insert Delete

4. Click on View and have the temperature vary from 700 to 900 K in increments of

50K. (Note that the step variable has units.) Then click on the start button.

Available Case Studies			-Case Studies Data	Selection		
Case Study 1	A <u>d</u> d		Curre <u>n</u> t Case Stud	dy Case Study 1	_	
	Delete		Object	Variable	Ind	D
	Delete		PFR Feed	Temperature		Г
	View		PFR Feed	Comp Molar Flow (E-Benzene)		
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🎽 Case Studies Setup - Mai	n				×
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	Variable	Low Bound	High Bound	Step Size	
	PFR Feed - Temperature	700.0	900.0	50.00	
		Setup Disp	lay Properties	/Failed State	s
A <u>d</u> d Dele	te <u>R</u> esults			St <u>a</u> rt	

The result is the following in graphical form. The alternative form is a table which could be copied to a spreadsheet for future graphing.

To place in a spreadsheet use the copy with labels feature:

Now you can examine the effect of many other variables such as pressure, heat duty etc.



Effect of Feed Temperature on Conversion P=1.378 bar

вз:





Submit at the end of class:

- 1. Answers to page 1 questions.
 - 1.1. Why are there heaters between each reactor. Sketch the temperature, pressure and composition profiles in these reactors.
 - 1.2. What would happen if the heat duty on each of the reactors was set to zero? To do this you must remove heater outlet temperature specifications and set the duty to zero.
 - 1.3. Examine the effect of varying the inlet temperature to the first reactor on the outlet compositions of this process.
 - 1.4. Examine the effect of varying the inlet pressure outlet compositions of this process.
- 2. Graphs showing the following:
 - 2.1. Effect of Feed Temperature on conversion at P_{inlet} =1.378 bar
 - 2.2. Effect of Feed Pressure on Conversion at Tinlet=880K
 - 2.3. Effect of heat duty on conversion (either 1 or both heaters)