**Aspen Plus PFR Reactors Tutorial using Styrene with Pressure Drop Considerations**

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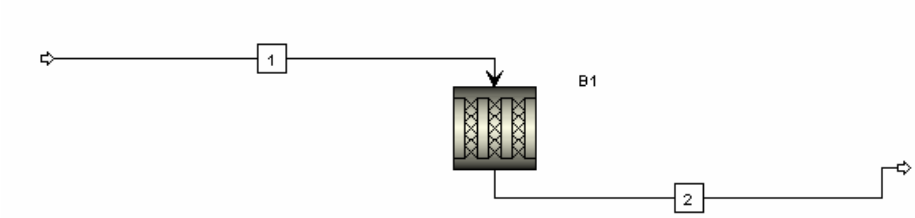
In this laboratory we will incorporate pressure-drop calculations into our Aspen Plus reactor models. We will use our ethylbenzene dehydrogenation problem in a plug flow reactor as a basis, and then add pressure drop. Since pressure drop correlations are not integral to this version of Aspen Plus, we'll incorporate them into the model using a pre-compiled Fortran subroutine which uses the Ergun equation. The laboratory computers do not have Fortran compilers – hence a pdrop.dll file has been provided for your use in this lab and in your reactor design project.

***Section 1***

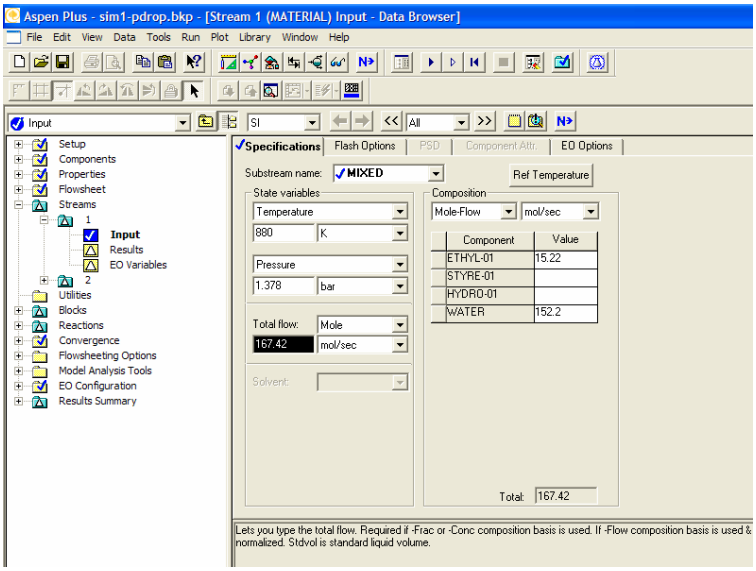
The first task is to set up your simulation directory, and store the pressure drop files appropriately so that Aspen Plus can access these files.

1. Create a directory for this pressure drop simulation on your H: drive and note the path to this directory. You might want to call it Aspen in the root directory on the H: drive.
2. Move the following files to this directory: pdrop.dll, pdrop.list, pdrop.lib and def.def.
3. Next open def.def using notepad, and modify the text line to specify your path as:
   DLOPT: H:*your directory path*\pdrop.list
   Save this file to the same directory.
4. Open pdrop.list using notepad, and modify the text line to specify your path as well as: H:*your directory path*\pdrop.dll. Save in the same directory.
5. Now we are ready to begin our Aspen Plus simulation.
6. Start Aspen 12.1.
7. Open a new case by choosing a blank simulation. (Do not use the templates for consistent units when specifying your kinetics. We will use SI units for all reactors with kinetics).
8. Choose *Data* from the main menu and click *Setup.* You can enter the title and brief description of the process by choosing the *Description* tab.
9. Select 'SI' units for both input and output results on the Global tab.
10. Under the Report Options, Stream tab, specify Mole and Mass for both the Flow Basis and the Fraction Basis.
11. Choose the *Components* option in the data browser window to start adding chemical components. Install the chemicals for a reactor: Styrene, ethyl benzene, hydrogen and water. Use the *Find* button to find the component ID and then add it.
12. Next, under *Properties, Specifications*, select your base property method. Since these compounds are hydrocarbons, use the Peng-Robinson thermodynamic package.
13. Install RPlug (Kinetic reactor). Using the Model Library, click on *Reactors* and then choose *RPlug*. Click on the *RPlug* icon, then release left mouse button. Move cursor to pfd screen and then press left mouse button only once.
14. To add streams, From the Model Library at the bottom of the Aspen Plus Process Flowsheet Window, select the *Material STREAMS* tab and click once. This will allow you to place multiple streams as needed. Move the cursor, now a crosshair, onto the process flowsheet. Click once, drag the cursor to connect the first stream to the feed port of your vessel (shown in red) and click again. You have just created stream 1.

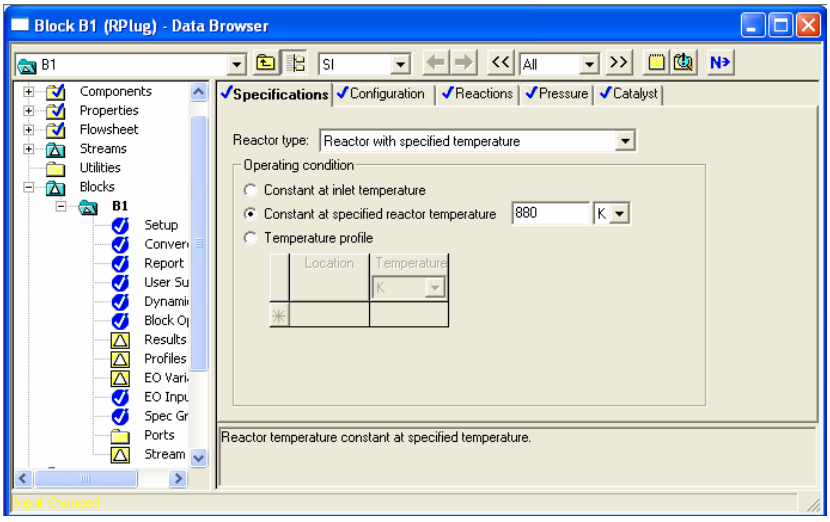
Add outlet stream to the reactor in a similar way.



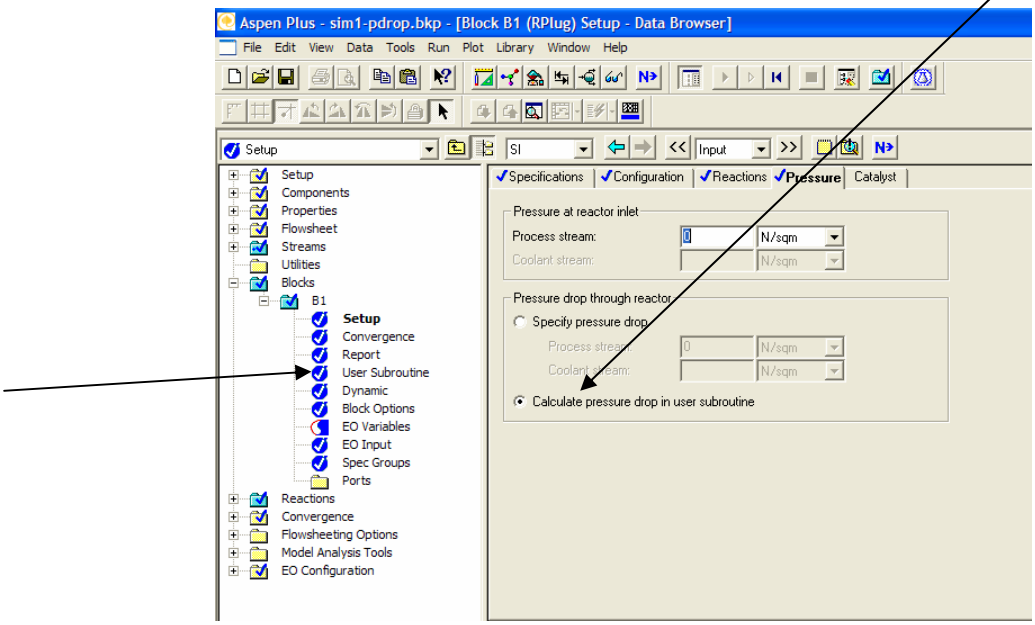

15. Specify the feed stream (Double click on the stream or right click on it and then choose input or through *Data, Streams* in the main menu) with a 10/1 ratio of steam:ethylbenzene. The total molar flow rate of 167.42 gmol/s (15.22 gmol/s ethylbenzene, 152.2 gmol/s water) at initial conditions of 880 K & 1.378 bar.




16. To input the reactor specifications, double click on the reactor block. The reactor Data Browser opens. Specify an isothermal reactor with the length and diameter of the reactor as 8 ft × 8 ft, respectively (for an 11.4 $m^3$ reactor).

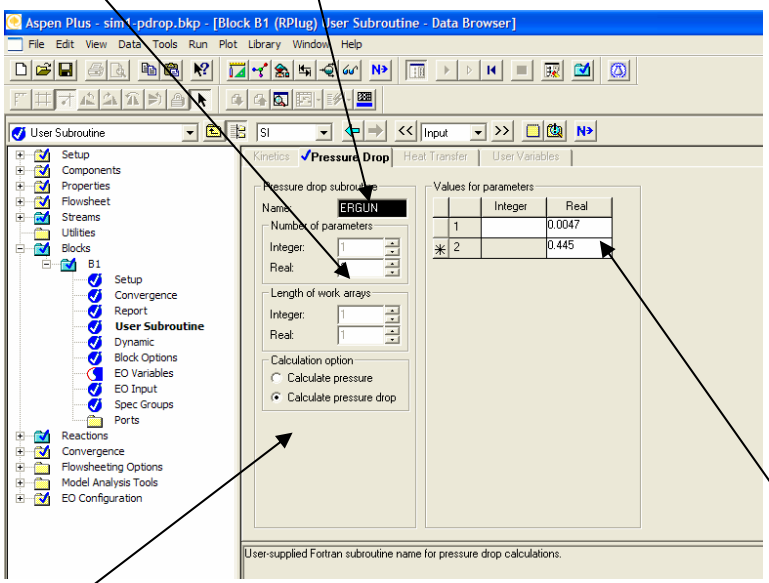


17. To specify the use of a User Subroutine for pressure drop calculations, select the Pressure tab and elect “Calculate pressure drop in user subroutine”.




18. Next select the User Subroutine entry in the data browser. Supply the name of the function as ‘ERGUN’. The user subroutine requires two catalyst parameters for its calculations. The first parameter is particle diameter in units of meters and the second parameter is catalyst bed void fraction. Select 4.7 mm for your particle size and 0.445 for your void fraction.

18.1. Click on the pressure drop tab and indicate that you’ll be specifying 2 real parameters.




18.2. Specify these parameters as .0047m particle diameter and 0.445 void fraction.

18.3. Indicate that you want to calculate pressure drop (not pressure) using this user routine.

19. Finally, you'll need to specify the reactions to complete the specification for the PFR.

19.1. Choose the *Reactions* block in the browser window. Then click on *Reactions.* Click *New* on the window that appears. A new dialog box opens, enter a reaction ID and specify the reaction as *Power Law.* Then click *Ok.*

19.2. For this simulation, consider only the forward rate for the reaction of

$$C_6H_5 - C_2H_5 \Leftrightarrow C_6H_5 - CH = CH_2 + H_2 \tag{1}$$

In this reactor we will neglect the aspect that reaction 1 is an equilibrium reaction and model this system using a power law expression. The reaction rate expression for the forward reaction is the same as that used in the Equilibrium reactor laboratory.

$$r_{EB} = -7.491\times10^{-2}\,\frac{\text{gmol EB}}{\text{g}_{\text{cat}}\text{s kPa}}\exp\left[-\frac{21874\ \text{cal/mol}}{\left(1.987\,\frac{\text{cal}}{\text{mol K}}\right)T}\right]\left(p_{EB}\right) \tag{1}$$

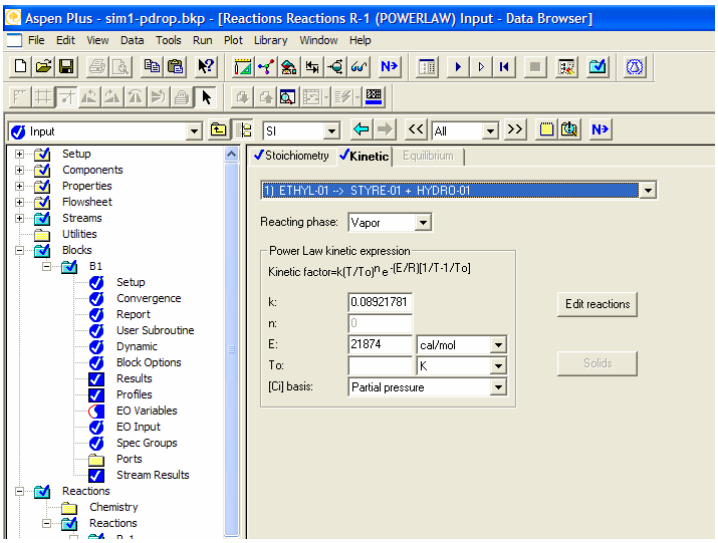
Notice that the reaction rate has units and that the concentration term is partial pressure with units of kPa.

Convert from units per ($g_{cat}$) to per reactor volume ($m^3$), using catalyst bulk density $\rho_{bulk}$ to convert the rate constant so that the units of the rate tranforms

from:
$$r_{cat}\ [=]\ \frac{\text{gmol}}{\text{s}-\text{gcat}} \tag{2}$$

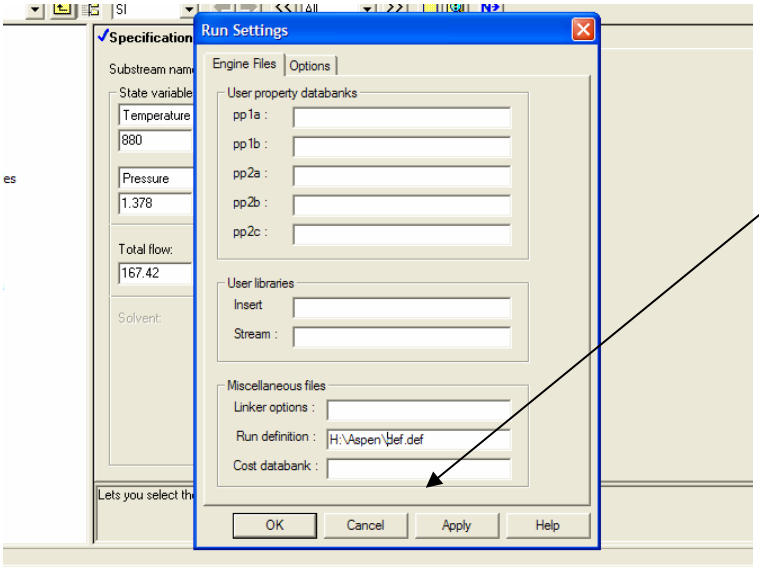
to:
$$r_{pseudo-\text{hom}ogeneous} = r_{cat}\cdot\rho_{bulk}\,[=]\frac{kmol}{m^3-s} \tag{4}$$

using:
$$\rho_{bulk} = 1191\ \text{kg}_{\text{cat}}/\text{m}^3_{\text{reactor}} \tag{5}$$




20. Go back to reactor specification, Reactions tab, and select this reaction set.

21. Finally, you'll need to direct Aspen Plus to the user subroutines. To do so, select, Run, Settings, and type H:*your directory name*\def.def in the Run definition field.




22. You are now ready to run your simulation.
23. Create a plot of Pressure as a function of reactor length (from the block profile screen).
***24.*** Export your results as an Aspen report file (*.rep). ***Hand in this report.***

***Section 2***

25. Next we'll compare these results to hand calculations and Polymath calculations.
    ***25.1.*** Do hand calculations for approximate pressure drop based on the Ergun Equation and the parameters provided in the attached pages. You should always do this calculation to check your Polymath program. ***Hand in these calculations.***
***26.*** Create your own Polymath model as shown in the next 4 pages using the parameters provided. ***Hand in a copy of the results.***

# Sample Calculations: Rxtr Pressure Drop

C. LaMarca

Rxtr Dimensions:

$D = 8' = 2.438\ m$
$L = 8' = 2.438\ m$
$V = 11.38\ m^3$

- Properties Based on 91% STEAM -

from DIPPR

$$\mu_{STEAM}\Big|_{880K} = 3.272e^{-5}\ kg/m\text{-}s$$

$$\bar{M}_w = \frac{18\ g\ W}{gmol\ W} \cdot \frac{0.91\ gmol\ W}{gmol\ T} + \frac{106.17\ g\ EB}{gmol\ EB} \cdot \frac{0.09\ gmol\ EB}{gmol\ TOT} = 25.94\ g/gmol$$

$$\bar{\rho}_o = \frac{P}{RT} \cdot \bar{M}_w = \frac{1.378e^5\ Pa}{8.314\ \frac{Pa\ m^3}{gmol\text{-}K}\ 880\ K} \cdot \frac{25.94\ g}{gmol} = 0.4885\ kg/m^3$$

$$\frac{dP}{dW} = \frac{-\beta_o}{A_c(1-\phi)\rho_c} \frac{P_o}{P}\left(\frac{T}{T_o}\right)\frac{F_T}{F_{TO}} \qquad (4\text{-}27)$$

$$\beta_o = \frac{G(1-\phi)}{\rho_o D_p \phi^3}\left[\frac{150(1-\phi)\mu}{D_p} + 1.75\,G\right] \qquad (4\text{-}25)$$

$$A_c G = F_{EB_o} MW_{EB} + F_W MW_W = \left[15.22\ \frac{gmol}{s}(106.17)\frac{g}{gmol} + 152.2\ \frac{gmol}{s}(18\ g/gmol)\right]\frac{kg}{1000}$$

$$A_c G = 4.3555\ kg/s$$

$$V_o = \frac{F_{T_o} RT}{P_o} = \frac{(15.22 + 152.2)\ gmol/s\ \ 8.314\ \frac{Pa\text{-}m^3}{gmol\text{-}k}\ 880\ K}{1.378e^5\ Pa}$$

$$V_o = 8.889\ m^3/s$$

$$G = \frac{4.3555\ kg/s}{\pi/4\,(2.438)^2} = 0.932998\ kg/m^2\text{-}s$$

$$\beta_o = \frac{0.932998\ kg/m^2\text{-}s\ (1-0.445)}{(.4885\ kg/m^3)(4.7\cdot10^{-3}m)(.445)^3}\left[\frac{150(1-.445)}{4.7\cdot10^{-3}\ m}\,3.27e^{-5}\frac{kg}{m\text{-}s} + 1.75\,\frac{.933}{m^2\text{-}s}\right.$$

$$= 2539\left[\tfrac{1}{s}\right]\left[0.596 + 1.633\right]\frac{kg}{m^2} = 5637.5$$

$$\frac{\beta_0}{A_c(1-\phi)\rho_c} = \frac{5637.5 \ kg/m^2\text{-}s^2}{\frac{\pi}{4}(2.438)^2 m^2 (1-.445)(2146.3 \ kg/m^3)} = 1.014 \ \frac{kg \ m^3}{m^2\text{-}s^2 \ m^2\text{-}kg}$$

$$P_a = \frac{N}{m} = \frac{kg \ m/s^2}{m^2} \qquad \frac{P_a}{kg} = \frac{1}{m\text{-}s^2} \hookrightarrow = 1.014 \ \frac{P_a}{kg}$$

PRESSURE DROP:

$$\frac{dP}{dW} = -1.014 \left[\frac{P_a}{kg}\right] \frac{P_0}{P} \frac{T}{T_0} \frac{F_T}{F_{T0}} \left(\frac{kg}{1000 g}\right) = 1.014 \cdot 10^{-3} \frac{P_a}{g} \frac{P_0}{P} \frac{T}{T_0} \frac{F_T}{F_{T0}}$$

MOLE BALANCES:

$$\frac{dF_{EB}}{dW} = -r_{EB}' \qquad F_T = F_{W0} + F_{EB} + F_S + F_H$$

$$\frac{dF_S}{dW} = r_S = -r_{EB}'$$

$$\frac{dF_H}{dW} = r_H = -r_{EB}'$$

$$P_{EB} = \frac{F_{EB}}{F_T} P\Big|_{W=0} = \left(\frac{15.22}{167.72}\right) 1.378e^5 \ Pa \ \frac{1 kPa}{10^3 Pa} = 12.5 \ kPa$$

$$P_0 = 1.378 \times 10^5 \ Pa = 137.8 \ kPa$$

Expected Catalyst wt. from Aspen:

$$V = 11.38 \ m^3$$

$$W = 11.38 \ \frac{(1-0.445) m^3_c}{m^3_{reactor}} \ \frac{2146 \ kg_c}{m^3_a} = 13553.9 \ kg$$

$$= 1.355 \cdot 10^7 g$$

$X = 90\%$

Isothermal = 880 K

CL

# Check on Pressure Drop

$$\frac{dP}{dW} \simeq -1.014 \cdot 10^{-3} \frac{Pa}{g}$$

$$\Delta P \simeq -1.014 \cdot 10^{-3} \left[\frac{Pa}{g}\right] (1.355 \cdot 10^{7} g) = 13740.2 \text{ Pa}$$

$$\left(\frac{13740.2}{1.378 \cdot 10^{5}}\right) 100 = 9.97\%$$

You should always do this calculation to check your Polymath Program.

$$\frac{dF_{EB}}{dW} = -F_{EB} \frac{dX_{EB}}{dW} \simeq -7.491 \cdot 10^{-2} \exp\left[\frac{-21874 \frac{cal}{gmol}}{1.987 \frac{cal}{gmol\,K} \cdot 880 K}\right] \frac{mol}{g\text{-}s\text{-}kPa} \cdot 12.5 kPa$$

Again using the highest possible rate at $W=0$ and $P_{EB}|_{max} = 12.5 kPa$

$$k(880K) = 2.764 \cdot 10^{-7} \frac{gmol}{g\text{-}s\text{-}kPa} \qquad r = 2.764 \cdot 10^{-7} \frac{gmol}{g\text{-}s\text{-}kPa} \cdot 12.5 kPa$$

$$= \underbrace{3.455 \cdot 10^{-6} \frac{gmol}{g\text{-}s}}$$

this is in Polymath output

$$Y_{EB} \simeq \frac{\left(2.764 \cdot 10^{-7} \frac{gmol}{g\text{-}s\text{-}kPa}\right)\left(1.355 \cdot 10^{7} g\right) 12.5 kPa}{15.22 \text{ gmol/s}}$$

$$= \frac{46,8}{15.22} = 3.08$$

This is ok, since the avg $P_{EB}$ will be less than 12.5 kPa

# POLYMATH Results
## Pressure Drop in Isothermal Styrene Reactor 02-23-2005, Rev5.1.230

## Calculated values of the DEQ variables

| Variable | initial value | minimal value | maximal value | final value |
|---|---|---|---|---|
| W | 0 | 0 | 1.355E+07 | 1.355E+07 |
| FEB | 15.22 | 0.972075 | 15.22 | 0.972075 |
| FS | 0 | 0 | 14.247925 | 14.247925 |
| FH | 0 | 0 | 14.247925 | 14.247925 |
| P | 1.378E+05 | 1.224E+05 | 1.378E+05 | 1.224E+05 |
| FW | 152.2 | 152.2 | 152.2 | 152.2 |
| T | 880 | 880 | 880 | 880 |
| k | 2.765E-07 | 2.765E-07 | 2.765E-07 | 2.765E-07 |
| FT | 167.42 | 167.42 | 181.66793 | 181.66793 |
| P0 | 1.378E+05 | 1.378E+05 | 1.378E+05 | 1.378E+05 |
| pEB | 12.527273 | 0.6546941 | 12.527273 | 0.6546941 |
| rEB | -3.463E-06 | -3.463E-06 | -1.81E-07 | -1.81E-07 |
| FT0 | 167.42 | 167.42 | 167.42 | 167.42 |
| Betacat | 0.001014 | 0.001014 | 0.001014 | 0.001014 |
| X | 0 | 0 | 0.9361317 | 0.9361317 |

## ODE Report (RKF45)

Differential equations as entered by the user
[1] d(FEB)/d(W) = rEB
[2] d(FS)/d(W) = -rEB
[3] d(FH)/d(W) = -rEB
[4] d(P)/d(W) = -Betacat*P0/P*FT/FT0

Explicit equations as entered by the user
[1] FW = 152.2
[2] T = 880
[3] k = 7.491e-2*exp(-21874/1.987/T)
[4] FT = FEB+FS+FH+FW
[5] P0 = 1.378e5
[6] pEB = FEB/FT*P/1000
[7] rEB = -k*pEB
[8] FT0 = 15.22+152.2
[9] Betacat = 1.014e-3
[10] X = (15.22-FEB)/15.22

Comments
[6] k = 7.491e-2*exp(-21874/1.987/T)
*mol/(gcat s kPa)*
[8] pEB = FEB/FT*P/1000
*kPa*
[13] Betacat = 1.014e-3
*Pa/g*

Independent variable
variable name : W
initial value : 0
final value : 13550000

Precision
Step size guess. h = 0.000001
Truncation error tolerance. eps = 0.000001
General
number of differential equations: 4
number of explicit equations: 10
Data file: C:\Rowan Design Project\2005 Aspen Models\Pressure Drop - reactor\styrene pressure drop-CL.pol

***Section 3***

27. Next, let's explore how the reactor aspect ratio (L/D) impacts the pressure drop for equal reactor volume (and hence reactor conversion).
    - 27.1. Calculate length and diameter parameters for equal volume reactor over the range of L/D from 0.1 – 5 in an Excel spreadsheet.
    - 27.2. Go back to your Aspen simulation and explore the pressure drop as a function of L/D. Record final pressure and kg of ethylbenzene in your effluent stream for each case. When the pressure drop gets too large, the program will have trouble converging, so begin at your lower L/D and increase to find the place where pressure drop becomes too great for the program to converge.
    - 27.3. Create a plot of $\Delta P$ vs. L/D, and ethylbenzene conversion vs L/D. ***Hand in these plots.***

***Section 4***

The adiabatic reactor configuration is the most common reactor used in the production of styrene. A radial flow pattern is used to minimize the pressure drop. In this reactor the catalyst is contained between 2 vertical cylindrical screens. The gas flows from the inner vertical cylinder, through the catalyst, to the outer cylinder. This radial flow design gives a large flow area and minimizes the pressure drop through the catalyst. The adiabatic dehydrogenation reaction process is the most common method and is licensed by Fina-Badger and Monsanto (ABB Lummus Crest).

Isothermal multitubular reactors are used by BASF in Europe and Asahi in Japan. These reactors in principle have the dual advantage of avoiding a very high temperature at the reactor inlet and maintaining a sufficiently high temperature at the reactor outlet. In practice these conditions are very difficult to achieve because of heat transfer problems. The multitubular reactor is very expensive and the required temperature of the heat transfer fluid exceeds the stable temperature of molten salts, used commonly in high temperature applications, and flue gas is used instead. This results in a gas-gas heat transfer coefficient which is much lower than the molten salt heat transfer coefficient.

Another technology is the StyroPlus process developed by UOP and implemented in a demonstration-scale by Mitsubishi Chemical in Japan (alternative name SMART). In this process the equilibrium is driven by burning hydrogen in a separate reactor following the ethylbenzene dehydrogenation reactor. This has the dual effect of increasing the gas temperature, from the combustion process, and removing the hydrogen to drive the equilibrium to higher conversions.[1]

28. In this section, we'll modify our Aspen model to describe a multi-tubular reactor.
    - 28.1. Assume a reactor of equal volume with tube length of 8'. If the tubes are 2" in diameter, calculate the number of tubes necessary to achieve this volume.
    - 28.2. In the Aspen reactor configuration sheet, select Multitube reactor and specify your calculated number of tubes.
    - 28.3. Run your simulation and generate a plot of Pressure vs reactor length. Compare this plot to the plot you generated in section 1, and comment on the differences. ***Hand in this plot and your comments.***

[1] Kirk-Othmer Encyclopedia of Chemical Technology. editorial board, Herman F. Mark *.et al.* ; 4th ed. New York, Wiley, c1991-. Vol 22 p 972 4th Ed.