

## Aspen Plus PFR Reactors Tutorial using Styrene with Pressure Drop

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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. This reaction system will be based on a feed containing a 10:1 ratio of steam:ethylbenzene at these conditions: 15.22 gmol/s ethylbenzene, 152.2 gmol/s water (steam) at initial conditions of 880 K & 1.378 bar.

### Section 1

- 1) First we'll perform hand calculations and Polymath calculations for our reaction system incorporating pressure drop.

#### Reaction Kinetics:

In this reactor we will neglect the aspect that reaction 1 is an equilibrium reaction and model this system using a power law expression for the forward reaction.

$$r = -k p_{EB} \quad (1)$$

where,

$$k = A \cdot \exp\left(-E^*/R^*T\right), \quad A = 7.491 \times 10^{-2} \frac{\text{gmol EB}}{\text{g}_{\text{cat}} \cdot \text{s} \cdot \text{kPa}} \quad \text{and} \quad E^* = 21874 \text{ cal / gmol}.$$

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

- 2) Convert to **SI** units on two bases:
  - a) First on per catalyst weight ( $\text{kg}_{\text{cat}}$ ) basis.
  - b) Second on per reactor volume ( $\text{m}^3$ ) basis.

Use catalyst bulk density  $\rho_{\text{bulk}}$  to convert the rate constant so that the units of the rate transforms

$$\text{from:} \quad A_{\text{cat}} \quad [=] \quad \frac{\text{gmol}}{\text{s} \cdot \text{g}_{\text{cat}}} \quad (1)$$

$$\text{to:} \quad A_{\text{pseudo-homogeneous}} = A_{\text{cat}} \cdot \rho_{\text{bulk}} \quad [=] \quad \frac{\text{kmol}}{\text{m}^3 \cdot \text{s}} \quad (3)$$

$$\text{using:} \quad \rho_{\text{bulk}} = 1191 \text{ kg}_{\text{cat}} / \text{m}_{\text{reactor}}^3 \quad (4)$$

**Hand in these units conversions with your lab.**

- 3) The following three pages illustrate the derivation of reaction rate expression for your reactor including the momentum balance for pressure drop. As you can see, we need to estimate fluid properties for your reaction mixture, and we need information about reactor dimensions and catalyst properties. Here we assume a bed void fraction of 0.445 and particle size of 4.7 mm. Assume our reactor dimensions are: L=D=8 ft.

- 4) Do your own Polymath calculations for the estimate of pressure drop based on the parameters provided as shown in the attached pages.

**You should always do this type of hand calculation to check your Polymath program.** Equations 1 – 5 form the basis of your model. You can use the hand-calculated value of  $\beta_0$  directly in Eqn. 5. If you do so for your memos, however, you must include the hand-calculated development, as shown below.

### Sample Calculations for Reactor Pressure Drop

Feed Conditions:

15.22 gmol/sec EB

152.2 gmol/sec H<sub>2</sub>O

T=880K; P=1.378 bar

Reactor Dimensions:

D=8 ft=2.438 m

L=8 ft=2.438 m

V=11.38 m<sup>3</sup>

Mole Balances:

$$\frac{dF_{EB}}{dW} = r_{EB}$$

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

$$\frac{dF_{H_2}}{dW} = r_{H_2} = -r_{EB}$$

$$F_T = F_{H_2O} + F_{EB} + F_S + F_{H_2}$$

(Eqns. 1—4)

Momentum Balance:

$$\frac{dP}{dW} = \frac{-\beta_0}{A_c(1-\phi)\rho_c} \frac{P_0}{P} \left( \frac{T}{T_0} \right) \frac{F_T}{F_{T0}}$$

$$\beta_0 = \frac{G(1-\phi)}{\rho_0 D_p \phi^3} \left[ \frac{150 \cdot (1-\phi)\mu}{D_p} + 1.75G \right]$$

$$A_c G = \dot{m} = F_{EB_0} M_{w-EB} + F_{H_2O_0} M_{w-H_2O} = 0.01522 \cdot 106.18 + 0.1522 \cdot 18 = 4.3557 \text{ kg/s}$$

$$G = \frac{4.3557 \text{ kg/s}}{\frac{\pi}{4} (2.438)^2 \text{ m}^2} = 0.932998 \text{ kg/m}^2 \cdot \text{s}$$

$$\text{and } (1-\phi)\rho_c = \rho_{bulk}$$

Using the properties based on 91% Steam (from DIPPR):

$$\mu_{\text{steam}}(880\text{K}) = 3.272e^{-5} \text{ kg/m-s}$$

$$\overline{M}_w = 18 \frac{\text{g}_{\text{H}_2\text{O}}}{\text{gmol}_{\text{H}_2\text{O}}} \cdot \frac{0.91 \text{ gmol}_{\text{H}_2\text{O}}}{\text{gmol}_T} + \frac{108.17 \text{ g}_{\text{EB}}}{\text{gmol}_{\text{EB}}} \cdot \frac{0.09 \text{ gmol}_{\text{EB}}}{\text{gmol}_T} = 25.94 \frac{\text{g}}{\text{gmol}}$$

$$\overline{\rho}_0 = \frac{P}{R \cdot T} \cdot \overline{M}_w = \frac{1.378e^5 \text{ Pa}}{8.314 \frac{\text{Pa} \cdot \text{m}^3}{\text{gmol} \cdot \text{K}}} \cdot 25.94 \frac{\text{g}}{\text{gmol}} = 0.4885 \frac{\text{kg}}{\text{m}^3}$$

$$\beta_0 = \frac{0.932998 \text{ kg/m}^2 \cdot \text{s} (1-0.445)}{0.4886 \text{ kg/m}^3 (4.7 \cdot 10^{-3} \text{ m}) \cdot (0.445)^3} \left[ \frac{150 \cdot (1-0.445)(3.27 \cdot 10^{-5} \text{ kg/m-s})}{4.7 \cdot 10^{-3} \text{ m}} + 1.75 \cdot 0.932998 \text{ kg/m}^2 \cdot \text{s} \right]$$

$$= 2539 \text{ s}^{-1} \cdot [0.5696 + 1.633] \text{ kg/m}^2 = 5637.5 \text{ kg/m}^2 \cdot \text{s}^2$$

so,

$$\frac{\beta_0}{A_c(1-\phi)\rho_c} = \frac{\beta_0}{A_c \rho_{\text{bulk}}} = \frac{5637.5 \text{ kg/m}^2 \cdot \text{s}^2}{\frac{\pi}{4} (2.438)^2 \text{ m}^2 \cdot 1191 \text{ kg}_{\text{cat}}/\text{m}^3} = 1.014 \frac{\text{kg/m}^2 \cdot \text{s}^2}{\text{kg}_{\text{cat}}} = 1.014 \frac{\text{Pa}}{\text{kg}_{\text{cat}}}$$

$$\frac{dP}{dW} = -1.014 \frac{\text{Pa}}{\text{kg}_{\text{cat}}} \frac{P_0}{P} \frac{T}{T_0} \frac{F_T}{F_{T_0}} \quad (\text{Eqn. 5})$$

Expected catalyst weight from reactor dimension and catalyst bulk density provide final condition:

$$V = \frac{\pi \cdot d_t^2}{4} \cdot L = \frac{\pi \cdot 2.438^2}{4} \cdot 2.438 = 11.38 \text{ m}^3$$

$$W = V \cdot \rho_b = 11.38 \text{ m}^3 \cdot 1191 \text{ kg}_{\text{cat}}/\text{m}^3 = 13559 \text{ kg}_{\text{cat}}$$

Approximate check on Pressure Drop Calculation:

$$\frac{dP}{dW} \approx \frac{\Delta P}{W} = -1.014 \text{ Pa/kg}_{\text{cat}}$$

$$\text{so, } \Delta P \approx -1.014 \text{ Pa/kg}_{\text{cat}} \cdot 13559 \text{ kg}_{\text{cat}} = -13749 \text{ Pa}$$

$$\text{and, } \frac{\Delta P}{P_0} = \frac{-13749}{1.378 \cdot 10^5} \approx 10\%$$

- 5) Create your own Polymath model using the parameters provided above. What units of rate constant should you use?
- 6) How do your Polymath results compare with the approximate hand calculations?
- 7) Plot pressure and ethylbenzene composition over the length of your reactor.

**Hand in a copy of the Polymath results and plot.**

## Section 2

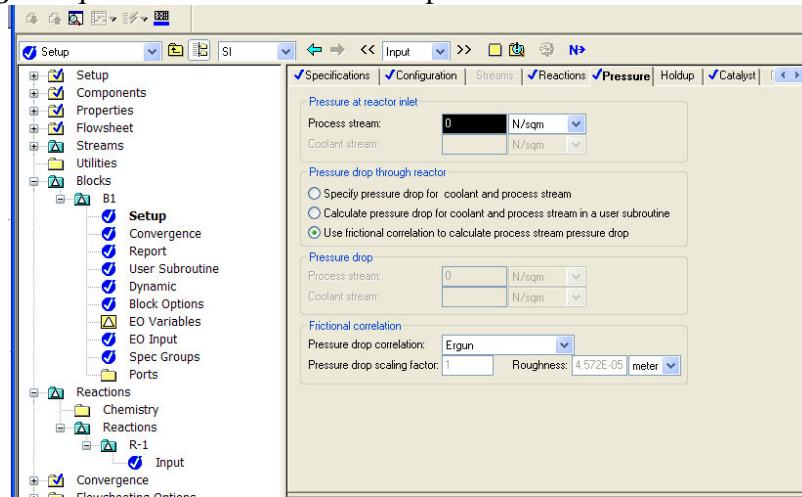
6. Start Aspen 13.2.
7. Open a new case by choosing a blank simulation.
8. Choose *Data* from the main menu and click *Setup*. You can enter the title and brief description of the process by choosing the *Description* tab.
9. Select 'SI' (**not MET**) units for both input and output results on the Global 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, ethylbenzene, 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 as we've done in previous labs (double click on the stream or right click on it and then choose input or through *Data, Streams* in the main menu), but in this case we will feed a mixture of steam and ethylbenzene 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 & 1.37 8 bar.
16. Specify the reactions for your system as considering only the forward rate for the reaction of



***Remember that your reaction is pseudo-first order in ethylbenzene partial pressure, so the power law exponent must be specified!***

17. Specify reaction kinetics using values derived in section 1. Select Reaction, *New*, and type, **General**. Create a new Power Law reaction specifying the stoichiometry on the *Configuration* tab.
18. On the kinetics tab, choose your reaction phase (vapor) and a partial pressure concentration basis. Select rate basis for your pre-exponential factor as catalyst weight – so use the A factor you calculated (in SI units) per kg-cat.
19. To input the reactor specifications, double click on the reactor block. The reactor Data Browser opens. Specify an isothermal reactor (Reactor with specified temperature, at constant inlet temperature). On the **Configuration** tab, specify the length and diameter of the reactor as 8 ft × 8 ft, respectively (for an 11.38 m<sup>3</sup> reactor).
20. As we saw in Section 1, pressure drop is a function of reactor dimensions, catalyst particle diameter and bed void fraction. For these calculations first select the **Pressure** tab.

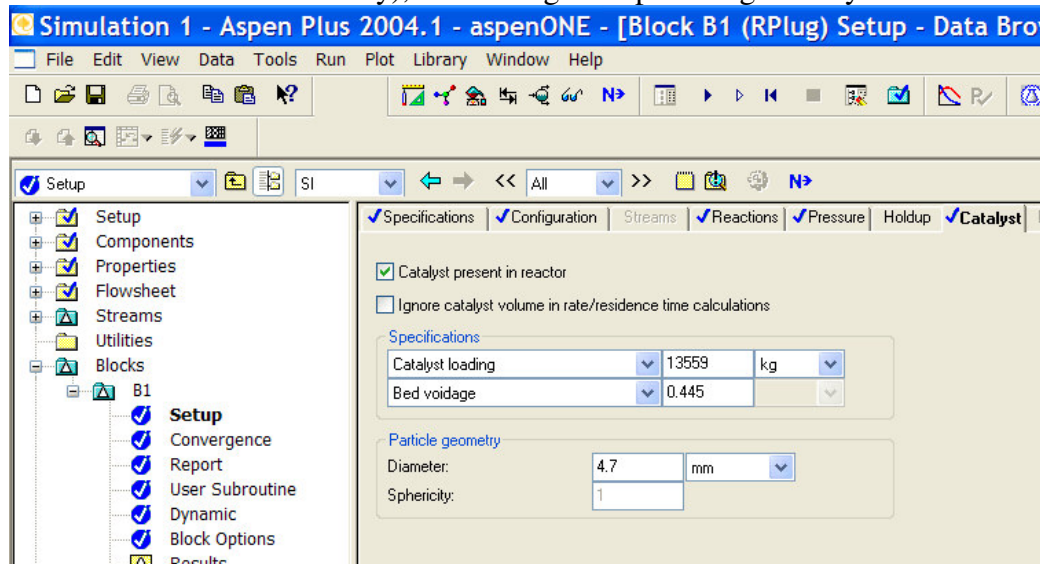
21. Select *Use frictional correlation to calculate the process stream pressure drop*. And, select the *Ergun* equation for the Pressure drop correlation:



22. Now we must specify catalyst properties.

22.1.1. First indicate that Catalyst is present in the reactor. (Do not select “Ignore catalyst volume in rate/residence time calculations”. This is only used if you specify reactor volume-based kinetics).

22.1.2. Next, specify catalyst loading (which you should calculate from reactor volume and bulk density), bed voidage and particle geometry.



23. Finally go to the Reactions tab, and select your reaction set.

24. Run your simulation. Examine results in the Reactor Profiles section. Tabulate the pressure and molar composition profiles in an Excel spreadsheet, as well as the Stream results.

25. Create a plot of Pressure and EB mol fraction as a function of reactor length.

**How do these results compare with your Polymath model?**

**Hand in this plot, the stream results and your comments with your lab.**

### Section 3

26. Next, let's explore how the reactor aspect ratio (L/D) impacts the pressure drop for equal reactor volumes (and hence reactor conversion).
  - 26.1. Try a reactor with 6.5 ft diameter and 12.12 ft length. Tabulate the  $\Delta P$ .
  - 26.2. Next, 10 ft diameter and 5.12 ft long. Again, tabulate the  $\Delta P$ .
  - 26.3. How about 6 ft diameter and 14.22 ft long? What happens?
  - 26.4. 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.<sup>1</sup>

27. In this section, we'll modify our Aspen model to describe an adiabatic multi-tubular reactor.
  - 27.1. Select reactor configuration of Adiabatic.
  - 27.2. Assume a reactor of equal volume ( $11.38 \text{ m}^3$ ) with tube length of 8'. If the tubes are 2" in diameter, calculate the number of tubes necessary to achieve this volume. ***Hand in this calculation.***
  - 27.3. In the Aspen reactor configuration sheet, select Multitube reactor and specify your calculated number of tubes.
  - 27.4. 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.***

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<sup>1</sup> 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.