CHME 312, Reaction Engineering, 2011 Spring

Exam II, Open Text (H. Scott Fogler, *Elements of Chemical Reaction Engineering*, 4th Ed.)

Note: For partial credit, please write your answer clearly and legibly.
For better credit, do all algebra and substitute digits, and check final figures carefully.

1. A homogeneous liquid phase second-order irreversible reaction

$$A + B \rightarrow C + D$$

is to be carried out in a PFR volume of 6.0 ft^3. It is proposed that to increase conversion, a CSTR of 100-gal capacity be installed just before the PFR. Calculate the **new conversion**. The values are given by $F_{A0} = F_{B0} = 1.50$ lbmol/hr, Temp. = 300 °F, $v_{A0} = v_{B0} = 4.5$ ft^3/hr, and X = 0.5. Assume that the reactors are operated isothermally. (50)

Sol)

- Mole Balance on the PFR: $V_{PFR} = F_{A0}\int_0^X \frac{dX}{-r_A}$

- Rate Law: $-r_A = kC_AC_B$

- Stoichiometry: Equal Molar $\Theta_B = 1$

$C_A = C_{A0}(1-X), C_B = C_{A0}(1-X)$

- Combine

$$V_{PFR} = \frac{F_{A0}X}{kC_{A0}^2(1-X)}$$

- Evaluate: rearrange to solve for k

$$k = \frac{F_{A0}X}{C_{A0}^2V_{PFR}(1-X)} = \left[\frac{v_0X}{C_{A0}V_{PFR}(1-X)}\right]$$

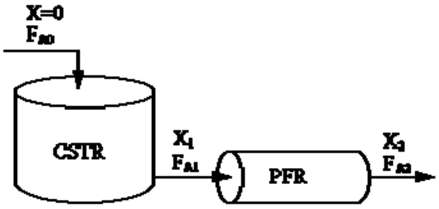
after mixing

$$v_0 = v_A + v_B = 4.5\ \text{ft}^3/\text{hr} + 4.5\ \text{ft}^3/\text{hr} = 9.0\ \text{ft}^3/\text{hr}$$

$$C_{A0} = \frac{F_{A0}}{v_0} = \frac{1.5\ \text{lbmol/hr}}{9.0\ \text{ft}^3/\text{hr}} = 0.167\ \text{lbmol/ft}^3$$

$$\therefore k = \frac{(9.0\ \text{ft}^3/\text{hr})(0.5)}{(0.167\ \text{lbmol/ft}^3)(6.0\ \text{ft}^3)((1-0.5)} = 8.98 \frac{\text{ft}^3}{\text{lbmol}\cdot\text{hr}}$$

Place CSTR before original PFR reaction



- Combine : $V_{CSTR} = \dfrac{F_{A0}X_1}{-r_{A1}}$
- Evaluate

$$V_{CSTR} = \frac{100\ \text{gal} \times 1\ \text{ft}^3}{7.48\ \text{gal}} = 13.37\ \text{ft}^3 = \frac{F_{A0}X_1}{-r_A} = \frac{F_{A0}X_1}{kC_{A0}^2(1-X_1)^2} = \frac{v_0 X_1}{kC_{A0}(1-X_1)^2}$$

$$V_{CSTR} = \frac{v_0 X_1}{kC_{A0}\left(1 - X_1\right)^2}$$

$$V_{CSTR} = \frac{v_0 X_1}{kC_{A0}\left(1 - 2X_1 + X_1^2\right)}$$

$$V_{CSTR}\, kC_{A0} - 2V_{CSTR}\, kC_{A0} X_1 + V_{CSTR}\, kC_{A0} X_1^2 = v_0 X_1$$

$$X_1^2 - \left(2 + \frac{v_0}{V_{CSTR}\, kC_{A0}}\right) X_1 + 1 = 0$$

$$X_1 = \frac{\left(2 + \dfrac{v_0}{V_{CSTR}\, kC_{A0}}\right) \pm \left[\left(2 + \dfrac{v_0}{V_{CSTR}\, kC_{A0}}\right)^2 - 4\right]^{1/2}}{2}$$

where $V_{CSTR} = 13.37\ \text{ft}^3, \text{k} = 8.98 \dfrac{\text{ft}^3}{\text{lbmol}\cdot\text{hr}}, C_{A0} = 0.167\ \text{lbmol/ft}^3, v_0 = 9.0\ \text{ft}^3/\text{hr}$

$$X_1 = \frac{\left(2 + \dfrac{9.0}{13.37 \times 8.98 \times 0.167}\right) \pm \left[\left(2 + \dfrac{9.0}{13.37 \times 8.98 \times 0.167}\right)^2 - 4\right]^{1/2}}{2}$$

$$= 0.52$$

$$V_{PFR} = F_{A0}\int_{X_1}^{X_2}\frac{dX}{kC_{A0}^2(1-X)^2} = \frac{v_0}{kC_{A0}}\int_{X_1}^{X_2}\frac{dX}{(1-X)^2} = \frac{v_0}{kC_{A0}}\left(\frac{1}{1-X_2}-\frac{1}{1-X_1}\right)$$

rearrange :

$$\frac{1}{1-X_2} = \frac{1}{1-X_1} + \frac{kC_{A0}V_{PFR}}{v_0}$$

where $X_1 = 0.52$, $V_{PFR} = 6.0\ \mathrm{ft}^3$, $k = 8.98\frac{\mathrm{ft}^3}{\mathrm{lbmol}\cdot\mathrm{hr}}$, $C_{A0} = 0.167\ \mathrm{lbmol/ft}^3$, $v_0 = 9.0\ \mathrm{ft}^3/\mathrm{hr}$

$$\frac{1}{1-X_2} = \frac{1}{1-0.52} + \frac{(8.98)(0.167)(6.0)}{9.0} = 2.08 + 1 = 3.08$$

X_2 = 1 - 1/3.08 = **0.675**

2. A is converted to B, C, and D according to the following reactions.

$$\begin{array}{lll} \mathrm{A}\rightarrow\mathrm{B} & r_B = k_1C_\mathrm{A}^{1/2} & k_1 = 0.05(\mathrm{mol/dm}^3)^{1/2}\cdot\mathrm{min} \\ \mathrm{A}\rightarrow\mathrm{C} & r_C = k_2C_\mathrm{A} & k_2 = 0.3/\mathrm{min} \\ \mathrm{A}\rightarrow\mathrm{D} & r_D = k_3C_\mathrm{A}^2 & k_3 = 0.24\mathrm{dm}^3/\mathrm{mol}\cdot\mathrm{min} \end{array}$$

Where the *k* values are specific reaction rates at 27°C. If the reaction is operated at 27°C and 4 atm with pure A entering of volumetric flow rate 10 dm^3/min. C is desired product and B and D are undesired product and are very costly to separate from B.

(a) **Sketch the instantaneous selectivities** ($S_{C/B}$, $S_{C/D}$, and $S_{C/BD} = r_C/(r_B + r_D)$) as a function of the concentration of C_A. (20)

$$S_{\mathrm{C/B}} = \frac{k_2}{k_1}C_\mathrm{A}^{1/2} = 60C_\mathrm{A}^{1/2}$$

$$S_{\mathrm{C/D}} = \frac{k_2}{k_3}\frac{1}{C_\mathrm{A}} = 1.25\frac{1}{C_\mathrm{A}}$$

$$S_{\mathrm{C/BD}} = \frac{k_2C_\mathrm{A}}{k_1C_\mathrm{A}^{1/2}+k_3C_\mathrm{A}^2} = \frac{0.3C_\mathrm{A}}{0.05C_\mathrm{A}^{1/2}+0.24C_\mathrm{A}^2}$$

- Since only C is desired the selectivity of C over B and D should be the maximum.

$\lim_{C_\mathrm{A}\to 0} S_{\mathrm{C/BD}} = 0$ and $\lim_{C_\mathrm{A}\to\infty} S_{\mathrm{C/BD}} = 0$

It has maximum value at $\frac{dS_{\mathrm{C/BD}}}{dC_\mathrm{A}} = 0$ or $C_\mathrm{A} = \left(\frac{k_1}{2k_2}\right)^{2/3}$

(b) What is the **conversion** of A in the first CSTR and how **many** CSTRs will be needed to get over 90% conversion for the process to be profitable? (30)

With k_1 and k_2 values given, $\mathbf{C_A = 0.221}$

$$C_{A0} = \frac{P}{RT} = \frac{8\text{atm}}{0.082\dfrac{\text{dm}^3\text{atm}}{\text{mol}\cdot\text{K}}\times 300\text{K}} = 0.326\text{mol/dm}^3$$

$$V_{CSTR1} = \frac{v_0(C_{A0}-C_A)}{-r_A} = \frac{v_0(C_{A0}-C_A)}{k_1C_A^{1/2}+k_2C_A+k_3C_A^2}$$

$$= \frac{10(0.326-0.221)}{(0.05)(0.221)^{1/2}+(0.3)(0.221)+(0.24)(0.221)^2} = \frac{1.05}{0.024+0.067+0.012} = 10.19\text{dm}^3$$

$$X_1 = \frac{(C_{A0}-C_{A1})}{C_{A0}} = \frac{0.326-0.221}{0.326} = 0.322$$

At 90% conversion $C_A = 1 - 0.9C_{A0} = 1 - (0.9)*(0.326) = 0.033$

For the 2nd reactor,

$$V_{CSTR2} = \frac{v_0(C_{A1}-C_{A2})}{-r_{A2}} = \frac{v_0(C_{A1}-C_{A2})}{k_1C_{A2}^{1/2}+k_2C_{A2}+k_3C_{A2}^2} = 10.19$$

$$1.019 = \frac{0.221-C_{A2}}{0.05C_{A2}^{1/2}+0.3C_{A2}+0.24C_{A2}^2}$$

By trial & error, $C_{A2} = 0.150$, likewise

$$V_{CSTR3} = \frac{v_0(C_{A2}-C_{A3})}{-r_{A3}} = \frac{v_0(C_{A2}-C_{A3})}{k_1C_{A3}^{1/2}+k_2C_{A3}+k_3C_{A3}^2} = 10.19$$

$$1.019 = \frac{0.150-C_{A2}}{0.05C_{A3}^{1/2}+0.3C_{A3}+0.24C_{A3}^2}$$

By trial & error, $C_{A3} = 0.101$, likewise

$$1.019 = \frac{0.101-C_{A3}}{0.05C_{A4}^{1/2}+0.3C_{A4}+0.24C_{A4}^2}$$

By trial & error, $C_{A4} = 0.066$, likewise

$$1.019 = \frac{0.066-C_{A4}}{0.05C_{A5}^{1/2}+0.3C_{A5}+0.24C_5}$$

By trial & error, $C_{A5} = 0.042$, likewise

$$1.019 = \frac{0.042-C_{A4}}{0.05C_{A5}^{1/2}+0.3C_{A5}+0.24C_5}$$

By trial & error, $\mathbf{C_{A6} = 0.026 < 0.033}$