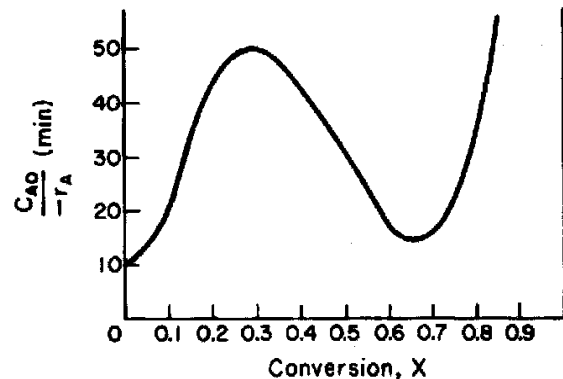


CHME 312, Reaction Engineering, Spring 2011

Exam I, 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, check final figures carefully.**

1. After graduation, suppose that you are working for a company of which business is to design and install reactors to process a liquid phase waste stream from the main plant. The reaction rate with conversion was observed and plotted as in the figure on the right. The concentration of interested material C_{A0} is often expressed in terms of molar flow rate per volumetric flow rate. Now you have 3 PFRs of volume 0.02, 0.03, and 0.06 m³ each and 3 MFRs (CSTRs) of volumes 0.02, 0.03, and 0.06 m³ each. Given volumetric flow rate of the waste, v , is 0.01 m³/min, find out the **optimum layout** of the reactors and estimate **final conversion**. (40)



Sol)

$$\text{Let } V_{P1} = 0.02\text{m}^3, V_{P2} = 0.03\text{m}^3, V_{P3} = 0.06\text{m}^3$$

$$V_{M1} = 0.02\text{m}^3, V_{M2} = 0.03\text{m}^3, V_{M3} = 0.06\text{m}^3$$

Liquid phase rxn, $v = v_0$

$$\text{- Design equation of PFR } V_P = \int_0^X \frac{F_{A0}}{-r_A} dX = \int_0^X \frac{C_{A0}v}{-r_A} dX = v \int_0^X \frac{C_{A0}}{-r_A} dX$$

$$\text{- Design equation of MFR } V_M = \frac{F_{A0}(X_{out} - X_{in})}{-r_A} = \frac{C_{A0}v(X_{out} - X_{in})}{-r_A}$$

- By $X = 0.3$, PFR is better than MFR

Area under curve to $X = 0.3$ (by Simpson rule of 3 points)

$$\begin{aligned} \text{Area} &= \frac{h}{3} \left[\frac{C_{A0}}{-r_A} \Big|_{X=0} + 4 \times \frac{C_{A0}}{-r_A} \Big|_{X=0.15} + \frac{C_{A0}}{-r_A} \Big|_{X=0.3} \right] \\ &= \frac{0.15}{3} (10 + 4 \times 30 + 50) = 9 \end{aligned}$$

$$\text{For PFR } V_P = (v)(\text{Area}) = (0.01)(9) = 0.09 \text{ m}^3 \Rightarrow V_{P2} + V_{P3} = 0.03\text{m}^3 + 0.06\text{m}^3$$

- By $X = 0.65$, MFR is better than PFR,

(However, we have given volumes of reactor and reaction rate between $X = 0.65$ and $X = 0.7$ changes only little, we can explore to $X = 0.7$ instead)

and with steep slope, large MFR is better to have smaller volume (or higher conversion)

Try with $V_{M3} = 0.06\text{m}^3$ and $X = 0.5$

$$V_M = \frac{C_{A0}v(X_{out} - X_{in})}{-r_A} = (v) \left(\frac{C_{A0}}{-r_A} \right)_{X=0.5} (0.5 - 0.3) = (0.01)(30)(0.2) = 0.06 \text{ OK}$$

Try with $V_{M2} = 0.03\text{m}^3$ and $X = 0.7$

$$V_M = \frac{C_{A0}v(X_{out} - X_{in})}{-r_A} = (v) \left(\frac{C_{A0}}{-r_A} \right)_{X=0.65} (0.7 - 0.5) = (0.01)(15)(0.2) = 0.03 \text{ OK}$$

- Now we have one PFR of $V_{P1} = 0.02\text{m}^3$ and one MFR of $V_{M1} = 0.02\text{m}^3$ left.

- For the rest range, PFR is much better than MFR.

- At the given curve, MFR \rightarrow PFR is better than PFR \rightarrow MFR (increasing rate of slope)

Conversion at the exit of MFR ($= 0.02\text{m}^3$)

$$\frac{0.02}{0.01} = \left(\frac{C_{A0}}{-r_A} \right)_{X_{M2}} (X - 0.7), \quad X = 0.77, \quad C_{A0}/(-r_A) \doteq 28$$

$$\left(\frac{C_{A0}}{-r_A} \right)_{X_{M2}} (X - 0.7) = (28)(0.07) = 1.96 \doteq 2 \Rightarrow X_5 = 0.77$$

Conversion at the exit of PFR

$$\frac{0.02}{0.01} = \int_{0.77}^X \left(\frac{C_{A0}}{-r_A} \right) dX$$

$$X = 0.83, \quad C_{A0}/(-r_A) \doteq 45$$

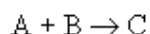
$$\int_{0.77}^X \left(\frac{C_{A0}}{-r_A} \right) dX = \frac{h}{3} \left[\frac{C_{A0}}{-r_A} \Big|_{X=0.77} + 4 \times \frac{C_{A0}}{-r_A} \Big|_{X=0.80} + \frac{C_{A0}}{-r_A} \Big|_{X=0.83} \right] \text{ OK}$$

$$= \frac{0.003}{3} (28 + 4 \times 33 + 45) = 0.02$$

**Reactor layout: ($V_{P2} = 0.03\text{m}^3$, $V_{P3} = 0.06\text{m}^3$) \rightarrow $V_{M3} = 0.06\text{m}^3$ \rightarrow $V_{M2} = 0.03\text{m}^3$
 \rightarrow $V_{M1} = 0.02\text{m}^3$ \rightarrow $V_{P1} = 0.02\text{m}^3$**

Final conversion = 0.83

2. The elementary, liquid-phase, irreversible reaction



is to be carried out in a flow reactor. Two reactors are available, a 600 dm^3 PFR that can only be operated at 300 K and a 200 dm^3 CSTR that can be operated up to 350 K . The two feed streams to the reactor mix to form a single feed stream that is equal molar in A and B, with a

total volumetric flowrate of 10 dm³/min. Estimate the operation temperature of CSTR at which it has the same conversion to the PFR? (30)

Additional Information: at 300 K, $k = 0.07 \text{ dm}^3/\text{mol}\cdot\text{min}$
 $E = 83140 \text{ J/mol}\cdot\text{K}$
 $C_{A0B} = C_{B0B} = 2 \text{ mol/dm}^3$ (before mixing)
 $v_{A0} = v_{B0} = 0.5 \cdot v_0 = 5 \text{ dm}^3/\text{min}$

Sol)

- Design equation of PFR

$$V_{\text{PFR}} = F_{A0} \int_0^X \frac{dX}{kC_{A0}^2(1-X)^2} = \frac{F_{A0}}{kC_{A0}^2} \int_0^X \frac{dX}{(1-X)^2} = \frac{F_{A0}}{kC_{A0}^2} \frac{X}{1-X}$$

$$\frac{kC_{A0}^2}{F_{A0}} V = \frac{X}{1-X}$$

$$v_{A0} = 5 \text{ dm}^3/\text{min}$$

Before mixing

$$C_{A0B} = 2 \text{ mol/dm}^3$$

$$F_{A0} = C_{A0B} \cdot v_{A0}$$

$$F_{A0} = (5 \text{ dm}^3/\text{min})(2 \text{ mol/dm}^3) = 10 \text{ mol/min}$$

After mixing

$$v_0 = v_{A0} + v_{B0} = 5 \text{ dm}^3/\text{min} + 5 \text{ dm}^3/\text{min} = 10 \text{ dm}^3/\text{min}$$

$$C_{A0} = 1 \text{ mol/dm}^3$$

$$C_{A0} = \frac{F_{A0}}{v_0} = \frac{10 \text{ mol/min}}{10 \text{ dm}^3/\text{min}} = 1 \frac{\text{mol}}{\text{dm}^3}$$

$$\frac{kC_{A0}}{F_{A0}} V = \frac{\left(0.07 \frac{\text{dm}^3}{\text{mol}\cdot\text{min}}\right) \left(1 \frac{\text{mol}}{\text{dm}^3}\right)^2 (600 \text{ dm}^3)}{\left(10 \frac{\text{mol}}{\text{min}}\right)} = 4.2 = \frac{X}{1-X}$$

$$X = \frac{4.2}{1+4.2} = 0.81$$

- Design equation for CSTR

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

$$k = \frac{F_{A0}X}{V_{CSTR}C_{A0}^2(1-X)^2} = \frac{\left(10 \frac{\text{mol}}{\text{min}}\right)(0.81)}{(200\text{dm}^3)\left(1 \frac{\text{mol}}{\text{dm}^3}\right)^2(1-0.81)^2} = 0.263$$

- At T $k = A \exp\left(-\frac{E}{RT}\right)$

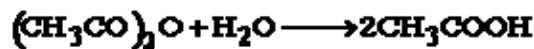
Divided by k value at 300 K

$$\frac{k}{k_{T=300}} = \exp\left[\left(\frac{E}{R}\right)\left(\frac{1}{300} - \frac{1}{T}\right)\right]$$

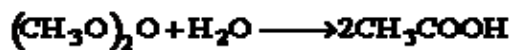
$$T = \frac{1}{\frac{1}{300} - \left(\frac{R}{E}\right)\ln\left(\frac{k}{k_{T=300}}\right)} = \frac{1}{\frac{1}{300} - \left(\frac{8.314}{83140}\right)\ln\left(\frac{0.263}{0.007}\right)} = 336.7 \text{ K}$$

Temperature of CSTR = 336.7 K

3. The hydrolysis of acetic anhydride is to be carried out at 25°C.

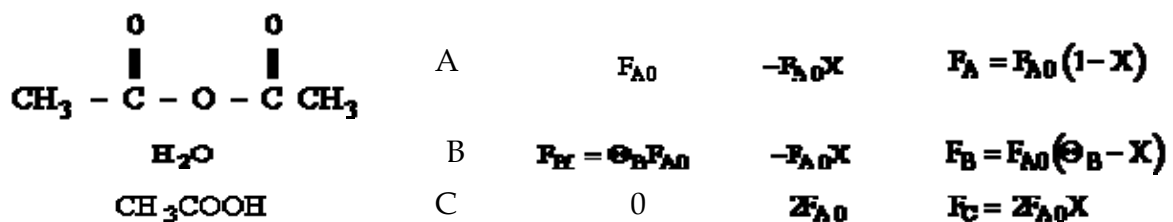


The water and acetic anhydride are mixed immediately before entering the reactor where the entering steam is 1 mole of acetic anhydride 51.2 mole of water. The volumetric feed rate of liquid is 0.003 dm³/s. The reaction rate constant, k', is 1.97x10⁻⁴ dm³/mol·s at 25°C with E = 12,000 cal/mol. Set up a stoichiometric table and determine the conversion achieved in a 0.5 dm³ PFR. (30)

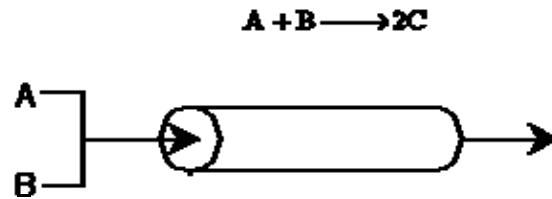


Sol)

- Stoichiometric table



- Conversion



a. Mole Balance/Design Equation

$$F_{A0} \frac{dX}{dV} = -r_A$$

b. Rate Law

$$-r_A = k' C_A C_B$$

3. Stoichiometry $v = v_0$

$$C_A = \frac{F_A}{v_0} = C_{A0}(1 - X)$$

$$C_B = C_{B0}(\Theta_B - X) \equiv C_{B0}$$

4. Combine

$$-r_A = k' C_A C_B = k C_A = \overbrace{k' C_{B0}}^k C_A = k C_{A0}(1 - X)$$

$$\frac{dX}{dV} = \frac{-r_A}{F_{A0}} = \frac{-r_A}{v_0 C_{A0}} = \frac{k C_{A0}(1 - X)}{v_0 C_{A0}}$$

$$\frac{dX}{dV} = \frac{k}{v_0}(1 - X)$$

$$\frac{dX}{1 - X} = \frac{k}{v_0} dV$$

$$k = k' C_{B0} = (1.97 \times 10^{-4} \text{ dm}^3/\text{mol}\cdot\text{s}) (51.2 \text{ mole}/\text{dm}^3) \\ = 0.01/\text{s}$$

$$V = 0 \quad X = 0$$

$$\ln \frac{1}{1 - X} = k \frac{V}{v_0}$$

$$X = 1 - \exp\left(-k \frac{V}{v_0}\right) = 1 - \exp\left(-\frac{(0.01)(0.5)}{0.003}\right) = \mathbf{0.81}$$