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Department of Chemical Engineering & Bio Technology

Assignment No.5

Subject: Chemical Reaction Engineering-I

Topic: Temperature & Pressure Effect & Non Ideal Flow

Q1. The acid-catalyzed irreversible (second order reaction) liquid-phase reaction $A \rightarrow R$ is carried out adiabatically in a CSTR. The reaction is second order in A. The feed, which is equimolar in a solvent (which contains the catalyst) and A, enters the reactor at a total volumetric flow rate of $10 \text{ dm}^3/\text{min}$ with the concentration of A being 4 mol/dm^3 . The entering temperature is 300 K .

(a) What CSTR reactor volume is necessary to achieve 80% conversion?

(b) What conversion can be achieved in a 1000 dm^3 CSTR? What is the new exit temperature?

(c) How would your answers to part (b) change, if the entering temperature of the feed were 280 K ? **Additional Information:** $\Delta H_{RX}(300\text{K}) = -3300 \text{ cal/mol}^\circ\text{C}$, $C_{PA} = C_{PB} = 15 \text{ cal/mol}^\circ\text{C}$, $C_{PS} = 18 \text{ cal/mol}^\circ\text{C}$, $K(300\text{K}) = 0.0005 \text{ dm}^3/\text{mol}\cdot\text{min}$, $E = 15,000 \text{ cal/mol}$

Q2. Determine the equilibrium conversion for the elementary reaction ($A \leftrightarrow R$) between 0°C and 100°C . (a) Construct a plot of temperature v/s conversion (b) What restriction should be placed on the reactor operating isothermally if conversion of 75% or highest is desired?

Additional Information at 298°K : $\Delta H_{RX} = -75300 \text{ J/mol}$, $C_{PA} = C_{PR} = \text{constant}$, $\Delta G^0 = -14130 \text{ J/mol}$

Q3. For a reversible first-order liquid-phase reaction ($A \leftrightarrow R$) with $-r_A = k_1 \cdot C_A - k_2 \cdot C_R$ is to be carried in plug flow reactor. For maximum permissible feed temperature of 95°C (maximum permissible operating temperature of 95°C) and the feed rate 1000 mol/min of reactant A, what is the optimum temperature progression in a plug flow reactor? A conversion of 80% is required and feed concentration of A is $C_{A0} = 4 \text{ mol/l}$ and $C_{R0} = 0$.

Also calculate the space time and volume needed for 80% conversion of a feed of $F_{A0} = 1000 \text{ mol/min}$ with $C_{A0} = 4 \text{ mol/l}$ and $C_{R0} = 0$

Additional Information: $k_1 = 34 \cdot 10^6 \exp(-48900/RT)$, min^{-1} and $k_2 = 1.57 \cdot 10^{18} \exp(-123800/RT)$, min^{-1} and E is in J/mol

Q4. A first order liquid-phase reaction ($A \rightarrow R$) is to be carried in mixed flow reactor. The density of reaction mixture is 1.2 g/cm^3 and specific heat is $0.9 \text{ cal/(g}^\circ\text{C)}$. The volumetric flow rate is $200 \text{ cm}^3/\text{s}$ and reactor volume is 10 liters. If the heat of reaction is -46000 cal/mol and feed temperature is 20°C , what are possible temperatures and conversions for stable, adiabatic operation for feed concentration of 4 mol/L ?

Additional Information: $k = 1.8 \cdot 10^5 \exp(-12000/RT)$, sec^{-1}

Q5. Dispersed non-coalescing droplets ($C_{A0} = 2 \text{ mol/liter}$) react ($A \rightarrow R$, $-r_A = k \cdot C_A^2$, $k = 0.5 \text{ liter/mol}\cdot\text{min}$) as they pass through a contactor. Find the average

concentration of A remaining in the droplets leaving the contactor if their RTD is given by the curve in Fig 1.

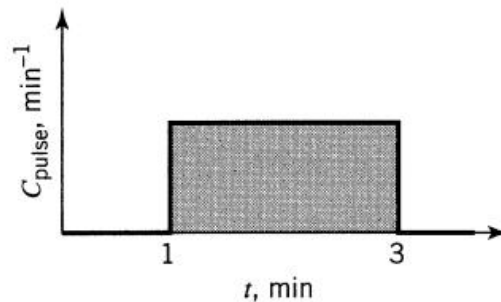


Figure 1. Concentration v/s time profile of macro fluid

Q6. The following data were obtained from a tracer test to a reactor.

| | | | | | | | | |
|--------------------------------|---|---|----|----|----|----|----|----|
| t(s): | 0 | 5 | 10 | 15 | 20 | 25 | 30 | 35 |
| $C_t(\text{mg}/\text{dm}^3)$: | 0 | 0 | 0 | 5 | 10 | 5 | 0 | 0 |

- 1) Plot $C_t(t)$.
- 2) Find $E(t)$.
- 3) Find the fraction of material that spends between 15 and 20 seconds in the reactor.
- 4) Find $F(t)$ and, the fraction of material that spends 25 seconds or less in the reactor.
- 5) Evaluate mean residence time.
- 6) Evaluate the variance.

Q7. The concentration data were observed a continuous response to a pulse input into a closed vessel. This vessel is to be used as reactor for decomposition of liquid A ($A \rightarrow R$, $-r_A = k \cdot C_A$ & $k = 0.10 \text{min}^{-1}$)

| t (min) | C_{pulse} (g/cm ³) | t (min) | C_{pulse} (g/cm ³) |
|---------|--|---------|--|
| 0 | 0 | 7 | 4 |
| 1 | 1 | 8 | 3 |
| 2 | 5 | 9 | 2.2 |
| 3 | 8 | 10 | 1.5 |
| 4 | 10 | 12 | 0.6 |
| 5 | 8 | 13 | 0.2 |
| 6 | 6 | 14 | 0 |

Calculate the conversion of reactant v/s t determine E.