Quiz-4

(a) for CSTR,

$$\tau = \frac{C_{A0} X_A}{(-r_A)}$$

$$-r_A = k_1 C_A - k_2 C_B = k_1 C_{A0}(1-X_A) - k_2 (C_{A0} X_A)$$

$$\tau = \frac{\cancel{C_{A0}} X_A}{\cancel{C_{A0}} [k_1 (1-X_A) - k_2 X_A]}$$

k_1 at 280 K :- $10^3 \exp\left(\frac{-2500}{280}\right) s^{-1} = 0.1325\ s^{-1}$

$$K = 7.8 = \frac{k_1 \text{ at } 280K}{k_2 \text{ at } 280K}$$

k_2 at 280K = 0.0169

$$\tau = \frac{X_A}{0.1325(1-X_A) - 0.0169 X_A}$$

$$600 = \frac{X_A}{0.1325 - 0.1494 X_A}$$

$$79.5 - 89.64 X_A = X_A$$

$\boxed{X_A = 0.877}$ @ 280K

Von't Hoff equation :-

b)

$$\ln\left(\frac{K_2}{K_1}\right) = \frac{-\Delta H_{rxn}}{R}\left[\frac{1}{T_2} - \frac{1}{T_1}\right]$$

$$\ln\left(\frac{K(T)}{K_{280}}\right) = \frac{+10 \frac{kcal}{mol}}{8.314\ J/mol\,K}\left[\frac{1}{480} - \frac{1}{280}\right]$$

$$\Delta H_{rxn} = \frac{-10 kcal}{mol} = -10 \times 4.184 \times 1000\ J/mol$$

$$= -41840\ J/mol$$

$$\ln\left(\frac{K_T}{K_{280}}\right) = \frac{+41840}{8.314}\left[\frac{-1}{672}\right] = -7.488$$

$$K_T = 0.0043 \text{ at } 480 K$$

$$k_1 \text{ at } 480K = 10^3 \exp\left(\frac{-2500}{480}\right) = 5.47\ s^{-1}$$

$$K_T = \frac{k_1}{k_2} = 0.0043$$

$$k_2 = \frac{5.47}{0.0043} = 1272.09\ s^{-1} \text{ at } 480K$$

$$\tau = 600 = \frac{X_A}{k_1(1-X_A) - k_2(X_A)}$$

$$600 = \frac{X_A}{5.47(1-X_A) - 1272.09 X_A}$$

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$$3282 - 766536 X_A = X_A$$

$$\boxed{X_A = 0.0042}$$

b) Energy balance:

$$0 = \dot{Q} + F_{A0} \sum_{i=1}^{n} \theta_i (H_{i0} - H_i) - \Delta H_{rxn}(T_f) F_{A0} X$$

$$C_p = 1000 \frac{cal}{kg \cdot K}$$

$$\frac{C_p \rho}{C_{A0}} = \frac{\cancel{1000}\ 1 \times \frac{kcal}{kg \cdot K} \times 1 \frac{kg}{L}}{5 \frac{mol}{L}}$$

$$\frac{C_p \rho}{C_{A0}} = 0.2 \frac{kcal}{mol \cdot K}$$

$$0 = \dot{Q} + F_{A0} \times 0.2 \times 10^3 (320 - 280) - (-10^4) \times F_{A0} \times \cancel{0.883}\ 0.877$$

$$\dot{Q} = -F_{A0} [8000 + 8770]$$

$$\dot{Q} = -\frac{C_{A0} V}{\tau} \times 16770$$

$$\frac{\dot{Q}}{V} = -139.75 \frac{cal}{L \cdot s}$$

Heat removed per liter of reactor volume to maintain at 280 K operating temperature.

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