P 11 - 5

Elementary gas phase reaction

$A \longrightarrow B + C$

Adiabatic ~~ga~~ PFR packed with catalyst

$v_0 = 20\ dm^3/s$

$P = 10$ ~~bar~~ atm

$T = 450\ K$

$C_{P_A} = 40\ J/mol \cdot K$

$C_{P_B} = 25\ J/mol \cdot K$

$C_{P_C} = 15\ J/mol \cdot K$

$$\left.\begin{aligned} H^\circ_A &= -70\ kJ/mol \\ H^\circ_B &= -50\ kJ/mol \\ H^\circ_C &= -40\ kJ/mol \end{aligned}\right\} @ 273\ K$$

$$k = 0.133 \exp\left[\frac{E}{R}\left[\frac{1}{450} - \frac{1}{T}\right]\right] \frac{dm^3}{kg\text{-}cat \cdot s}$$

$E = 31.4\ kJ/mol$

a) Conversion Vs T

$W_{max} = 50$ kg

$\Delta P = 0$

$A \longrightarrow B + C$

Species balance:

$$\frac{dx}{dW} = \frac{-r_A'}{F_{A0}} \qquad \text{— } 1$$

Stoichiometry:

$$C_A = C_{A0}\left(\frac{1-x}{1+\epsilon x}\right)\frac{T}{T_0}$$

$\epsilon = 1 \quad (y_{A0}\delta)$

$$C_A = C_{A0}\left(\frac{1-x}{1+x}\right)\frac{T}{T_0} \qquad \text{— } 2$$

rate law:

$$-r_A = k\,C_A \; ; \; k = 0.133 \exp\left[\frac{31400}{R}\left[\frac{1}{450} - \frac{1}{T}\right]\right] \qquad \text{— } 3$$

$\Delta H_{rx} = -20000$ J/mol

Energy balance:

$$T = T_0 + \frac{X\left[-\Delta H_{rx}(T_0)\right]}{\sum \Theta_I C_{p_I} + X \Delta C_p}$$

$$\Delta C_p = 15 + 25 - 40 = 0$$

$$T = T_0 + \frac{20000\,X}{40}$$

$$T = 450 + 500\,X \quad \text{— } 4$$

substituting 2, 3, and 4 in 1

$$\frac{dX}{dW} = \frac{-kC_A}{F_{A_0}}$$

$$= \frac{C_{A_0}}{(C_{A_0} v_0)}\, k \left(\frac{1-X}{1+X}\right) \times \left(\frac{T}{T_0}\right)$$

$$\frac{dW}{dX} = \left[\frac{v_0}{k}\right]\left[\frac{T}{T_0}\right]\left[\frac{1+X}{1-X}\right] \quad \text{— } 5$$

Need to solve this ODE for X from 0 → 1

at X = 0 W = 0

b) → Solve 5 with different T_o

c) Let

$$\frac{U_a}{\rho_b} = 0.08 \quad \frac{J}{s \cdot kg \cdot cat\ K}$$

ρ_b : bulk density kg/m^3

U_a = overall heat transfer coefficient $J/s\,m^2 K$

a : sp. heat exchange area (m^2/m^3)

For isothermal operations,
$\dot{Q}$ term is added to energy balance

$$\frac{dT}{dW} = \frac{\frac{Ua}{\rho}(T_a - T) + r'_A(-\Delta H_{rxn})}{F_{A0}\, C_{pA}} \quad - (6)$$

T_a = ~~323 K~~ 293 K

Equation (5) and (6) needs to be solved simultaneously.

$$\frac{dT}{dW} = 0 \Rightarrow \underline{\underline{\dot{Q} = -r'_A(-\Delta H_{rxn})}}$$

d) For pressure drop following extra equations are added.

$$\frac{dP}{dW} = -\frac{\alpha}{2}\left(\frac{T}{T_0}\right)\left(\frac{P_0}{P/P_0}\right)(1+\epsilon x)$$

$$C_A = C_{A0}\left(\frac{1-x}{1+\epsilon x}\right)\frac{T}{T_0}\,\frac{P}{P_0}$$