

P 11 - 5

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Elementary gas phase reaction



Adiabatic ~~gas~~ PFR packed with catalyst

$$v_0 = 20 \text{ dm}^3/\text{s}$$

$$P = 10 \text{ bar atm}$$

$$T = 450 \text{ K}$$

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

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

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

$$H_A^\circ = -70 \text{ kJ/mol}$$

$$H_B^\circ = -50 \text{ kJ/mol}$$

$$H_C^\circ = -40 \text{ kJ/mol}$$

} @ 273 K

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

$$E = 31.4 \text{ kJ/mol}$$

a) Conversion Vs T

$$W_{max} = 50 \text{ kg}$$

$$\Delta P = 0$$



Species balance:

$$\frac{dx}{dW} = \frac{-r_A'}{F_{A0}} \quad \text{--- (1)}$$

Stoichiometry:

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

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

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

rate law:

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

$$\Delta H_{rx} = -20000 \text{ J/mol} \quad \text{--- (3)}$$

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Energy balance :

$$T = T_0 + \frac{x [-\Delta H_{rx}(T_0)]}{\sum \theta_i C_{p_i} + x \Delta C_p}$$

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

$$T = T_0 + \frac{20000 x}{40}$$

$$T = 450 + 500 x \quad \text{--- (4)}$$

substituting (2), (3), and (4) in 1

$$\frac{dx}{dW} = \frac{-k C_A}{F_{A_0}}$$

$$= \frac{C_{A_0}}{(C_{A_0} V_0)} k \left( \frac{1-x}{1+x} \right) \times \left( \frac{T_0}{T} \right)$$

$$\frac{dW}{dx} = \left[ \frac{V_0}{k} \right] \left[ \frac{T}{T_0} \right] \left[ \frac{1+x}{1-x} \right] \quad \text{--- (5)}$$

Need to solve this ODE for  
 x from 0 → 1

at x = 0    W = 0

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b) → solve 5 with different  $T_0$

c) Let

$$\frac{Ua}{P_b} = 0.08 \frac{J}{s \cdot kg \cdot cat \cdot K}$$

$P_b$  : bulk density  $kg/m^3$

$Ua$  = overall heat transfer coefficient  $J/s \cdot m^2 \cdot K$

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

For isothermal operations,

$\dot{Q}$  term is added to energy balance

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

$$T_a = \cancel{323} = 293 \text{ K}$$

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.

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

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