CROCIO Tut 1.5 2019

→ Liquid-phase
→ elementary
→ autocatalytic reaction → irreversible
→ semi-batch reactor

$$A + B \rightarrow 2B$$

$k = 0{,}25\ L/mol \cdot min$

$V_0 = 1L$ (Pure A)

$C_{A0} = 5\ mol/L$

$C_{B0} = 5\ mol/L$ (added at $5mL/min$) @ $C_B = 5\ mol/L$

$$r_A = -kC_AC_B \quad \text{-- (1)}$$

$$r_B = -r_A \quad \text{-- (2)}$$

Species A:

M.B.: $F_{A0}^{\nearrow 0} - F_A^{\nearrow 0} + r_AV = \frac{dN_A}{dt} = \frac{d(C_AV)}{dt}$

$$r_AV = V\frac{dC_A}{dt} + C_A\frac{dV}{dt} \quad \text{-- (3)}$$

Overall species mass balance:

$$\rho_0Q_0 - 0 + 0 = \frac{d\rho V}{dt}$$

assume constant density system $\therefore \rho_0 = \rho$

$$\therefore \boxed{\frac{dV}{dt} = Q_0} \quad \text{-- (4)}$$

$$\Rightarrow \int_{V_0}^{V} dV = Q_0 \int_0^t dt$$

$$\therefore \quad V = V_0 + Q_0 t \qquad (5)$$

Subs. eq (4) into eq. (3)

$$\therefore \quad r_A V = V\frac{dC_A}{dt} + C_A Q_0$$

$$\Rightarrow \frac{dC_A}{dt} = r_A - \frac{Q_0 C_A}{V} \qquad \text{---} (6)$$

$$\Rightarrow \boxed{\frac{dC_A}{dt} = -kC_A C_B - \frac{Q_0 C_A}{V}} \qquad (7)$$

Species B:

M.B.: $F_{B_0} - \cancel{F_B}^{\,0} + r_B V = \frac{dN_B}{dt} = V\frac{dC_B}{dt} + C_B\frac{dV}{dt}$

$$C_{B_0} Q_0 + r_B V = V\frac{dC_B}{dt} + C_B\frac{dV}{dt}$$

But $\frac{dV}{dt} = Q_0$

$$\therefore \quad V\frac{dC_B}{dt} + C_B Q_0 = r_B V + C_{B_0} Q_0$$

$$\frac{dC_B}{dt} = r_B + \frac{Q_0(C_{B_0} - C_B)}{V}$$

$$\Rightarrow \boxed{\frac{dC_B}{dt} = kC_A C_B + \frac{Q_0(C_{B_0} - C_B)}{V}} \qquad (8)$$

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Time to completion:

$$N_{A0} = C_{A0} \cdot V_0$$

$$= \frac{5 mol}{L} \times 1L = 5 mol \rightarrow$$

∴ 5 mol B is required.

Rate B is added $= C_B Q_0$

$$= \frac{5 mol}{L} \cdot \frac{0,05 L}{min}$$

$$= 0,25 \frac{mol}{min} \rightarrow$$

Time to completion $= 5 mol \cdot \frac{min}{0,25 mol}$

$$= 20 min \rightarrow$$

Using python:

$$r_{A max} = -1,56 \, mol A / L \cdot min \rightarrow$$

This is observed at $t = 2,63$ mins $\rightarrow$