# P8.4

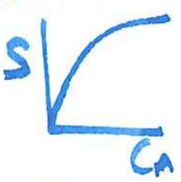
a)

$$A \rightarrow X \qquad +r_X = k\, C_A^{1/2}$$

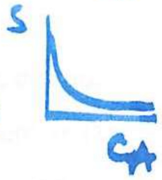
$$A \rightarrow B \qquad +r_B = k_2\, C_A$$

$$A \rightarrow Y \qquad r_Y = k_3\, C_A^{2}$$

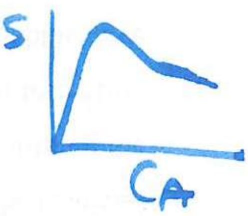
1) $$S_{B/X} = \frac{r_B}{r_X} = \frac{k_2 C_A}{k_1 C_A^{1/2}} = \frac{k_2}{k_1} C_A^{1/2}$$




2) $$S_{B/Y} = \frac{r_B}{r_Y} = \frac{k_2 C_A}{k_3\, C_A^{2}} = \frac{k_2}{k_3 C_A}$$




3) $$S_{B/XY} = \frac{r_B}{r_X + r_Y} = \frac{k\, C_A}{k_1 C_A^{1/2} + k_3 C_A^{2}}$$




b) Volume of first reactor

⇒ we need to maximize $S_{B/XY}$.

~~Max $S_B$~~ Max $S_{B,XY} = 10$ @ $C_A^* = 0.04$ mol/dm³

So a CSTR should be used with exit concentration of $C_A^*$

$$C_{A0} = \frac{P_A}{RT} = 0.162 \ \frac{mol}{dm^3}$$

$$-r_A = r_X + r_B + r_Y = k_1 C_A^{1/2} + k_2 C_A + k_3 C_A^2$$

$$\therefore \ V = \frac{v_0 (C_{A0} - C_A^*)}{-r_A} = \sout{92.4}\ 92.81 \ dm^3$$

c)

$$\tau = 9.24 \ min$$

$$\tau = \frac{C_B}{r_B} \Rightarrow C_B^* = 0.11 \ \frac{mol}{dm^3}$$

$$\tau = \frac{C_X}{r_X} \Rightarrow C_X^* = 0.007 \ \frac{mol}{dm^3}$$

$$\tau = \frac{C_Y}{r_Y} \Rightarrow C_Y^* = 0.0037 \ \frac{mol}{dm^3}$$

d)

$$X = \frac{C_{A0} - C_A}{C_{A0}}$$

$$= \sout{0.74}\ 0.75$$

e) CSTR followed by PFR, $X = 0.99$

Mole balance : $dX/dV = F_{A0}/-r_A$

$$V = \left[ \int_{0.74}^{0.99} \frac{dX}{-r_A} \right] \times 10 \times 0.162 = \sout{92.8}\ 91.18 \ dm^3.$$

f)

$E_2$ is the smallest activation energy

+ve ✓ $\Rightarrow$ higher selectivity at lower temp.

-ve × $\Rightarrow$ $r_B$ decreases → production of B ↓

Need to compromise between high Selectivity and production.

We need expressions for $k_1$, $k_2$, and $k_3$

$$k_i = A_i e^{-E_i/RT}$$

Constant given temperature T = 300 K

$$\therefore A_1 = \frac{0.004}{\exp\left[\frac{-20000}{1.98(300)}\right]} = 1.49 \times 10^{12}$$

similarly,

$$A_2 = 5.79 \times 10^{6}$$

$$A_3 = 1.798 \times 10^{21}$$

Mole balance of species A

$$V = \frac{F_{A0} - F}{-r_A}$$

$$V = \frac{\upsilon (C_{A0} - C_A)}{-r_A}$$

$$\therefore \tau = \frac{C_{A0} - C_A}{k_1 C_A^{1/2} + k_2 C_A + k_3 C_A^2} \quad \text{——} \ (1)$$

Mole balance on other species

$$F_i = \upsilon C_i = r_i V$$

$$C_i = \tau r_i \quad \text{——} \ (2)$$

⇒ We can solve this system of nonlinear equations numerically.