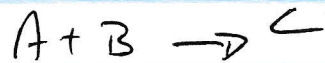


= CRO410 Tutorial 2.1 2019



- Elementary
- irreversible
- liquid
- Adiabatic
- equimolar feed @ 27°C (300.15 K)
- $Q = 1 \text{ L/s}$
- $C_{A0} = 0.1 \text{ mol/L}$

- $\Delta H_R = -6 \text{ kcal/mol}$: Exothermic
- $C_{pA} = C_{pB} = 15 \text{ cal/(mol}\cdot\text{K)}$
- $C_{pC} = 30 \text{ cal/(mol}\cdot\text{K)}$

→ $k = 0.01 \text{ L/(mol}\cdot\text{s)}$ at 300 K

→ $E = 10000 \text{ cal/mol}$ $\left| \frac{4187 \text{ J}}{\text{cal}} \right| \frac{\text{KJ}}{1000 \text{ J}} = 41.87 \frac{\text{KJ}}{\text{mol}}$ →

	<u>IN</u>	<u>A</u>	<u>OUT</u>	
A:	C_{A0}	$-C_{A0}X$	$C_{A0}(1-X)$	$= C_A$
B:	C_{B0}	$-C_{A0}X$	$C_{B0} - C_{A0}X$	$= C_B$
C:	0	$+C_{A0}X$	$C_{A0}X$	$= C_C$
			<u>$C_{A0} + C_{B0} - C_{A0}X$</u>	

$$r_A = -k C_A C_B \quad (\text{elementary})$$

$$r_B = r_A$$

$$r_C = -r_A$$

$$k_0 = k e^{E/RT} \quad (\text{at } 300 \text{ K})$$

2/

a) PFR

$$\frac{dF_A}{dV} = r_A$$

$$Q \frac{dC_A}{dV} = -k C_A C_B$$

$$-Q C_{A0} \frac{dX}{dV} = -k_0 e^{-E/RT} C_{A0}(1-X)(C_{B0} - C_{A0}X)$$

$$Q \frac{dX}{dV} = k_0 e^{-E/RT} C_{A0}(1-X)^2$$

$$\boxed{\frac{dX}{dV} = \frac{k_0 e^{-E/RT}}{Q} C_{A0}(1-X)^2} \quad \dots \textcircled{1}$$

* Since there is only one reaction in Adiabatic system:

$$T = T_0 + \frac{(-\Delta H_{rx}) (F_{A0}/G)}{\sum_i F_{i0} C_{p,i}} X_A$$

where $\sum_{i=1}^n F_{i0} C_{p,i} = F_{A0} C_{pA} + F_{B0} C_{pB} = 2 F_{A0} C_{pA}$

$$\therefore \boxed{T = T_0 - \frac{\Delta H_{rx}}{2 C_{pA}} X_A} \quad \dots \textcircled{2}$$

3/11

CSTR:

$$F_{A0} - F_A = -r_A V$$

$$F_{A0} - (F_{A0} - F_{A0}X) = k_0 e^{-E/RT} C_{A0}(1-X)(C_{B0} - C_{A0}X) V$$

$$F_{A0}X = k_0 e^{-E/RT} C_{A0}^2 (1-X)^2 V$$

$$Q C_{A0}X = k_0 e^{-E/RT} C_{A0}^2 (1-X)^2 V$$

$$X = \frac{k_0 e^{-E/RT} C_{A0} (1-X)^2 V}{Q} \quad \text{--- (3)}$$

$$V = \frac{X Q e^{E/RT}}{C_{A0}(1-X)^2 k_0}$$

Using python:

$$V_{PFR} = 302,22 \text{ L}$$

$$V_{CSTR} = 173,7 \text{ L}$$

4 //

b.) $T_a = 550k$
 $X = 1$

$$T_o = T + \frac{\Delta H_{rx} X}{2 C_p A} = 350k \quad (\text{python})$$

c.) See python

d.) → Using `fsolve` in python, the maximum conversion in a single 500L CSTR is 92,14%.

→ For 2 x CSTR of 250L

$$X(1^{st} 250L) = 88,13\% \quad \text{and} \quad X(2^{nd} 250L) = 75,35\%$$

$$\text{Total } X(2 \times 250L) = \underline{\underline{97,11\%}}$$

Note: Outlet for first 250L CSTR is at 476.42K. It needs to be cooled to at least 350K before being fed to second 250L CSTR.