CRE 410 Tutorial 2.1 2019

$$A + B \rightarrow C$$

- Elementary
- irreversible
- liquid
- Adiabatic
- equimolar feed @ 27°C (300.15 K)
- $Q = 2\ L/s$
- $C_{A0} = 0{,}1\ mol/L$

- $\Delta H_R = -6\ kcal/mol$ ∴ Exothermic
- $C_{pA} = C_{pB} = 15\ cal/(mol.K)$
- $C_{pC} = 30\ cal/(mol\,K)$

- $k = 0.01\ L/(mol.s)$ at 300k
- $E = 10\,000\ cal/mol \left| \frac{4{,}187\ J}{cal} \right| \frac{kJ}{1000\ J} = 41{,}87\ \frac{kJ}{mol}$ →

	In	Δ	OUT	
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	$+C_{A0}X$	$C_{A0}X$	$= C_C$
			$C_{A0} + C_{B0} - C_{A0}X$	

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

$$r_B = r_A$$

$$r_C = -r_A$$

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

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a) PFR

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

$$Q\frac{dC_A}{dV} = -kC_AC_B$$

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

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

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

(*) Since there is only one reaction in Adiabatic system:

$$T = T_0 + \frac{(-\Delta H_{Rx})(F_{A0}/G)}{\Sigma_i F_{i0} C_{pi}} X_A$$

where $\sum_{i=1}^{\hat{}} F_{i0} C_{pi} = F_{A0}C_{pA} + F_{B0}C_{pB} = 2F_{A0}C_{pA}$

$$\therefore \boxed{T = T_0 - \frac{\Delta H_{Rx}}{2C_{pA}} X_A} \quad \text{--- (2)}$$

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CSTR:

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

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

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

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

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

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

Using python:

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

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

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b.) $T_{ss} = 550k$

$X = 1$

$$T_0 = T + \frac{\Delta H_{rx} X}{2 GPA} = 350k \quad (python)$$

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

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

Total $X(2 \times 250L) = 97,1\%$.

Note: Outlet for first 250L CSTR is at 477.42k. It needs to be cooled to at least 350k before being fed to second 250L CSTR.