CR0410 STI 2019

Q1

$$A + B \rightarrow C$$

- irreversible, liquid
- $V_1 = V_2 = 2000\ L$
- $Q_{B1} = 3\ L/s$
- $C_{A0} = C_{B0} = 5\ mol/L$
- $C_{I0} = 5\ mol/L$
- $T_0 = 350\ K$
- $UA_1 = 3000\ W/K$, T_a is constant
- 2nd reactor is adiabatic
- reaction is elementary
- $r_A = -k C_A C_B$
- $k_0 = 1500\ L/(mol.s)$
- $E = 65000\ J/mol$
- $\Delta H_{Rx} = -60000\ J/mol_{Rx}$ (exothermic)
- $C_{pA} = 100\ J/(mol.K)$
- $C_{pB} = 70\ J/(mol.K)$
- $C_{pC} = 170\ J/(mol.K)$
- $C_{pI} = 60\ J/(mol.K)$
- $X_{TOT.} = 0,93$

	IN	Δ	OUT
A	F_{A0}	$-F_{A0}X$	$F_{A0}(1 - X)$
B	F_{B0}	$-F_{A0}X$	$F_{A0}(1 - X)$
C	0	$+F_{A0}X$	$F_{A0}X$
I	F_{I0}	—	F_{I0}

2/11

$$r_A = -k C_A C_B$$

$$r_A = -k_0 e^{-E/RT} \cancel{F_{A0}^2}(1-X)^2$$

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

$$r_B = r_A$$

$$r_C = -r_A$$

mol balance:

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

$$F_{A0} - (F_{A0} - X_1 F_{A0}) = k_0 e^{-E/RT} C_{A0}^2 (1-X_1)^2 V$$

$$C_{A0} Q_0 X_1 = k_0 e^{-E/RT} C_{A0}^2 (1-X_1)^2 V$$

$$\Rightarrow \boxed{X_1 = \frac{k_0}{Q_0} e^{-E/RT} C_{A0} (1-X_1)^2 V} \quad (1)$$

Energy balance:

$$\Delta \dot{H}_f = \Phi = UA(T_0 - T) = UAT_0 - UAT$$

$$\sum_{i=1}^{n} F_{i0} C_{pi0} (T-T_0) = \left(2F_{A0} C_{pA} + F_{I0} C_{pi}\right)(T-T_0)$$

$$= 2F_{A0} C_{pA} T + F_{I0} C_{pI} T - 2F_{A0} C_{pA} T_0 - F_{I0} C_{pi} T_0$$

$$(-\Delta F_A)\Delta H_{Rx} = F_A - \Delta H_{Rx} X_1$$

$$\sum_i F_{i0} C_{pi0}(T-T_0) + (-\Delta F_A)\Delta H_{Rx} = UA(T_0 - T)$$

$$(2F_{A0} C_{pA} + F_{I0} C_{pI} + UA)T + F_{A0}\Delta H_{Rx} X = (2F_{A0} C_{pA} + F_{I0} C_{pi})T_0 + UAT_0$$

Let $a = 2F_{A0} C_{pA} + F_{I0} C_{pI} + UA$

$$\Rightarrow \boxed{T_1 = \frac{(2F_{A0} C_{pA} + F_{I0} C_{pI})T_0}{a} + \frac{(UAT_0 - F_{A0}\Delta H_{Rx} X_1)}{a}} \quad (2)$$

CSTR1 Graph:

let $G = \frac{k_0 e^{-E/RT} C_{A0} V}{Q_0}$

$\therefore \quad X_1 = G(1-X_1)^2$

$\Rightarrow \boxed{X_1^2 - \frac{(2G+1)}{G} X_1 + 1 = 0}$ mol balance

energy balance:

$$\boxed{X_1 = \frac{a}{(UA T_0 - F_{A0} \Delta H_{rx})} T_1 - \frac{(2 F_{A0} C_{pa} + F_{I0} C_{pI})}{(UA T_0 - F_{A0} \Delta H_{rx})} T_0}$$

3

CSTR 2

IN	Δ	O-T
$F_{A0_2} = F_{A_0}(1-X_1)$	$-X_2 F_{A0_2}$	$F_{A_0}(1-X_1)(1-X_2)$
$F_{B0_2} = F_{A0_2}$	$-X_2 F_{A0_2}$	$F_{A_0}(1-X_1)(1-X_2)$
$F_{I0_2} = F_{I_0}$	—	F_{I_0}

$$r_{A_2} = -k C_A C_B$$

$$C_{A_2} = C_{A0_2}(1-X_2) = C_{A_0}(1-X_1)(1-X_2)$$
$$C_{B_2} = C_{A0_2}(1-X_2) = C_{A_0}(1-X_1)(1-X_2)$$

$$\therefore \quad r_{A_2} = -k_0 e^{-E/RT} C_{A_0}^2 (1-X_1)^2 (1-X_2)^2$$
$$r_{B_2} = r_{A_2}$$
$$r_{C_2} = -r_{A_2}$$

$$F_{A0_2} - F_{A_2} = -r_{A_2} V$$

$$F_{A0_2} X_2 = F_{A_0}(1-X_1)X_2 = C_{A0} Q_0 (1-X_1) X_2$$

$$\Rightarrow \quad \boxed{X_2 = \frac{k_0}{Q_0} e^{-E/RT_2} C_{A_0}(1-X_1)(1-X_2)^2 V} \quad (3)$$

$$T_{0_2} = T_1 \; ; \; \Sigma F_{i_0} C_{p_0} = 2\left(F_{A_0}(1-X_1)\right) C_{p_A} + F_{I0_2} C_{p_I}$$

$$\boxed{T_2 = T_1 - \frac{\Delta H_{RX} F_{A_0}(1-X_1)}{\left(2F_{A_0}(1-X_1)C_{p_A} + F_{I0_2} C_{p_I}\right)} X_2}$$

4

CSTR2 Graph:

Let $G = \frac{k_0}{Q_0} e^{-E/RT_2} C_{A_0}(1-X_1)V$

$\therefore \quad X_2 = G(1-X_2)^2$

$\Rightarrow$ $\boxed{X_2^2 - \frac{(2G+1)}{G} X + 1 = 0}$ mol balance.

and:

$$\boxed{X_2 = (T_1 - T_-)\left[\frac{2F_{A_0}(1-X_1)C_{p_A} + F_{I_{0_2}} C_{p_I}}{\Delta H_{RX} F_{A_0}(1-X_1)}\right]}$$

↳ energy balance.

6.) Q is constant. CSTR is at S.S. and medium is liquid

$T_0 = 642 K$
$T_1 \approx 556,06 K$
$T_2 \approx 696,05 K$

$X_1 = 60,65\%$
$X_2 = 82,23\%$
$X_{total} = 93\%$