CR0410 STI 2019

Q1

$$A + B \rightarrow C$$

→ irreversible, liquid
→ $V_1 = V_2 = 2000\ L$
→ $Q_0 l = 3\ L/s$
→ $C_{A0} = C_{B0} = 5\ mol/L$
→ $C_{I0} = 5\ mol/L$
→ $T_0 = 350\ K$
→ $UA_1 = 3000\ W/K$, 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}	$-F_{A0}X$	$F_{A0}(1 - \cancel{F_{A0}}X)$
B	F_{B0}	$-F_{A0}X$	$F_{A0}(1 - \cancel{F_{A0}}X)$
C	0	$+F_{A0}X$	$F_{A0}X$
I	F_{I0}	—	F_{I0}

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$$r_A = -k C_A C_B$$
$$r_A = -k_o e^{-E/RT} \underline{F_{Ao}}^2 (1-X)^2$$

$$r_A = -k_o e^{-E/RT} C_{Ao}^2 (1-X)^2$$
$$r_B = r_A$$
$$r_C = -r_A$$

<u>mol balance:</u>

$$F_{Ao} - F_A = -r_A V$$
$$F_{Ao} - (F_{Ao} - X_1 F_{Ao}) = k_o e^{-E/RT} C_{Ao}^2 (1-X_1)^2 V$$
$$C_{Ao} Q_o X_1 = k_o e^{-E/RT} C_{Ao}^2 (1-X_1)^2 V$$

$$\Rightarrow \boxed{X_1 = \frac{k_o}{Q_o} e^{-E/RT} C_{Ao} (1-X_1)^2 V} \quad (1)$$

<u>Energy balance:</u>

$$\Delta \dot{H}_f = \dot{Q} = UA(T_U - T) = \underline{UAT_U - UAT}$$

$$\sum_{i=1}^{n} F_{io} C_{pio} \overset{(T-T_o)}{=} (2F_{Ao} C_{pA} + F_{Io} C_{pi})(T - T_o)$$

$$= \underline{2F_{Ao} C_{pA} T + F_{Io} C_{pI} T - 2F_{Ao} C_{pA} T_o - F_{Io} C_{pi} T_o}$$

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

$$\sum_i F_{io} C_{pio} (T - T_o) + (-\Delta F_A)\Delta H_{Rx} = UA(T_U - T)$$

$$(2F_{Ao} C_{pA} + F_{Io} C_{pI} + UA)T + F_{Ao} \Delta H_{Rx} X = (2F_{Ao} C_{pA} + F_{Io} C_{pi}) T_o + UAT_U$$

Let $a = 2F_{Ao} C_{pA} + F_{Io} C_{pI} + UA$

$$\Rightarrow \boxed{T_1 = \frac{(2F_{Ao} C_{pa} + F_{I} C_{pI}) T_o}{a} + \frac{(UAT_U - F_{Ao} \Delta H_{Rx} X_1)}{a}} \quad (2)$$

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CSTR 2

IN	Δ	OUT
$F_{Ao2} = F_{Ao}(1-X_1)$	$-X_2 F_{Ao2}$	$F_{Ao}(1-X_1)(1-X_2)$
$F_{Bo2} = F_{Ao2}$	$-X_2 F_{Ao2}$	$F_{Ao}(1-X_1)(1-X_2)$
$F_{Io2} = F_{Io}$	$-$	F_{Io}

$$r_{A2} = -k C_A C_B$$

$$C_{A2} = C_{Ao2}(1-X_2) = C_{Ao}(1-X_1)(1-X_2)$$
$$C_{B2} = C_{Ao2}(1-X_2) = C_{Ao}(1-X_1)(1-X_2)$$

$$\therefore \quad r_{A2} = -k_o e^{-E/RT} C_{Ao}^2(1-X_1)^2(1-X_2)^2$$
$$r_{B2} = r_{A2}$$
$$r_{C2} = -r_{A2}$$

$$F_{Ao_2} - F_{A_2} = -r_{A_2} V$$

$$F_{Ao_2} X_2 = F_{Ao}(1-X_1)X_2 = C_{Ao}\, Q_o(1-X_1)X_2$$

$$\Rightarrow \boxed{X_2 = \frac{k_o}{Q_o} e^{-E/RT_2} C_{Ao}(1-X_1)(1-X_2)^2} \quad (3)$$

$$T_{o2} = T_1$$

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$$\sum_i F_i C_{p_i} = 2 F_{A0_2} C_{pA} + F_{I0_2} C_{pI}$$

$$= 2\left(F_{A0}(1-X_1)\right) C_{Ap} + F_{I0_2} C_{pI}$$

$$\Rightarrow \boxed{T_2 = T_{0_2} - \frac{\Delta H_{Rx} F_{A0}(1-X_1) X_2}{\left(2 F_{A0}(1-X_1) C_{pA} + F_{I0_2} C_{pI}\right)}}$$

b.) CSTR operate under steady-state conditions.
In liquid reactions, assuming system density is constant, Q has to be constant.

$T_0 \approx 833 K$
$T_1 \approx 565 k$ (out of CSTR1)
$T_2 \approx 612,4 k$ (out of CSTR2)

$T_2 > T_1 > T_0$ (as it should be)

$X_1 = 86,09\%$
$X_2 = 49,88\%$

$X_{tot} = 93\%$