CRG410 Tut 2.2 2019

$$A \rightarrow 3$$

- 1st order, liquid phase reaction
- Adiabatic CSTR
- $C_{A0} = 0{,}1$ mol/L
- $V = 500$ L
- $k_0 = 20\,000$ 1/s
- $E_a = 55\,000$ J/mol
- $\Delta H_{RX} = -30\,000$ J/mol (exothermic)
- $C_{pA} = C_{pB} = 157{,}9$ J/(mol.K)
- $Q = 2$ L/s

a) $T_0 = 340$K, calculate X

$$r_A = -k_0 e^{-E_a/RT} C_A$$

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

$$r_B = -r_A$$

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

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

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

$$\therefore \boxed{X = \frac{k_0 e^{-E_a/RT}}{Q}(1-X)V} \quad \text{---} \quad (1)$$

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

Conversion = 93,32 % (see Python)

or 2,2 %

↳ depends on 1st Guess

* For the X vs T based on energy balance, use:

$$X = \frac{C_{pA}(T - T_0)}{-\Delta H_{rx}} \quad \text{(② rearranged)}$$

b.) Change Q to 0,8 L/s.

Conversion = 97,72 %.

c.) $\Delta T_0 = 20\,K$

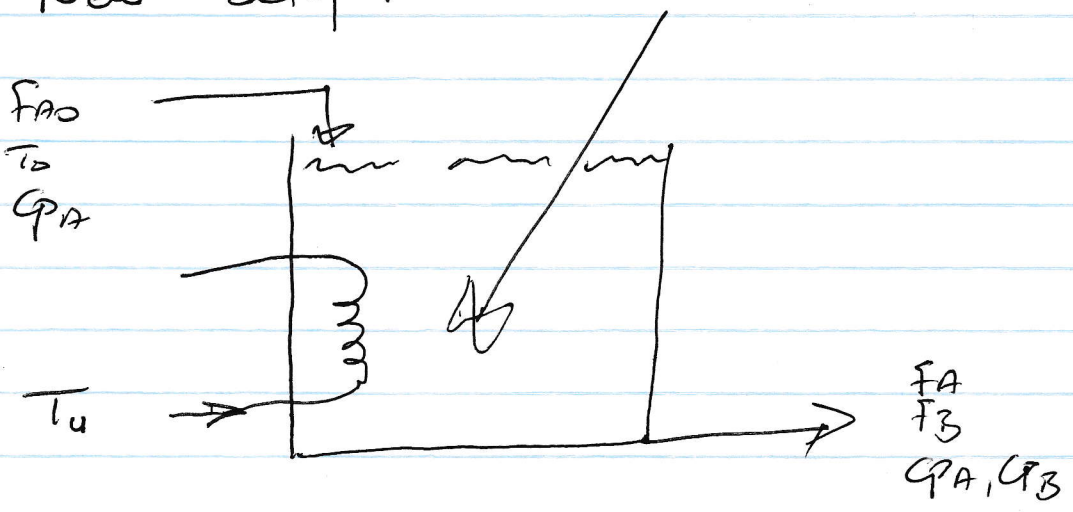
See python.

d) $E_{a\,new} = 60\,000\ J/mol$

See python, New conversion is 0,31 %.

More energy will be needed now to overcome the new activation energy

e.) New setup:



Energy Balance:

$$\Delta \dot{H}_{Fs} = Q = UA(T_u - T)$$

$$\therefore F_{A_0} C_{pA}(T - T_0) + (-\Delta F_A)\Delta H_{Rx} = UA(T_u - T)$$

$$F_{A_0} C_{pA} T - F_{A_0} C_{pA} T_0 + F_{A_0} X \Delta H_{Rx} = UAT_u - UAT$$

$$T(F_{A_0} C_{pA} + UA) - F_{A_0} C_{pA} T_0 + F_{A_0} \Delta H_{Rx} X = UAT_u$$

$$T = \left(\frac{F_{A_0} C_{pA}}{F_{A_0} C_{pA} + UA}\right) T_0 + \frac{UAT_u - F_{A_0}\Delta H_{Rx} X}{(F_{A_0} C_{pA} + UA)}$$

let $a = C_{A_0} Q C_{pA} + UA$

$$\therefore \boxed{T = \frac{C_{A_0} Q C_{pa} T_0}{a} + \frac{UAT_u - C_{A_0} Q \Delta H_{Rx}}{a} X}$$

$$T_{adiabatic} = T_0 - \frac{\Delta H_{Rx}}{C_{pA}} X$$

$$X_{EB} = \frac{C_{A_0} Q C_{pA} T_0}{C_{A_0} Q \Delta H_{Rx}} + \frac{UAT_u - aT}{C_{A_0} Q \Delta H_{Rx}}$$

$$\boxed{X_{EB} = \frac{C_{pA} T_0}{\Delta H_{Rx}} + \frac{(UAT_u - aT)}{C_{A_0} Q \Delta H_{Rx}}}$$

$T_u = 513.9\,K$ (see Python)