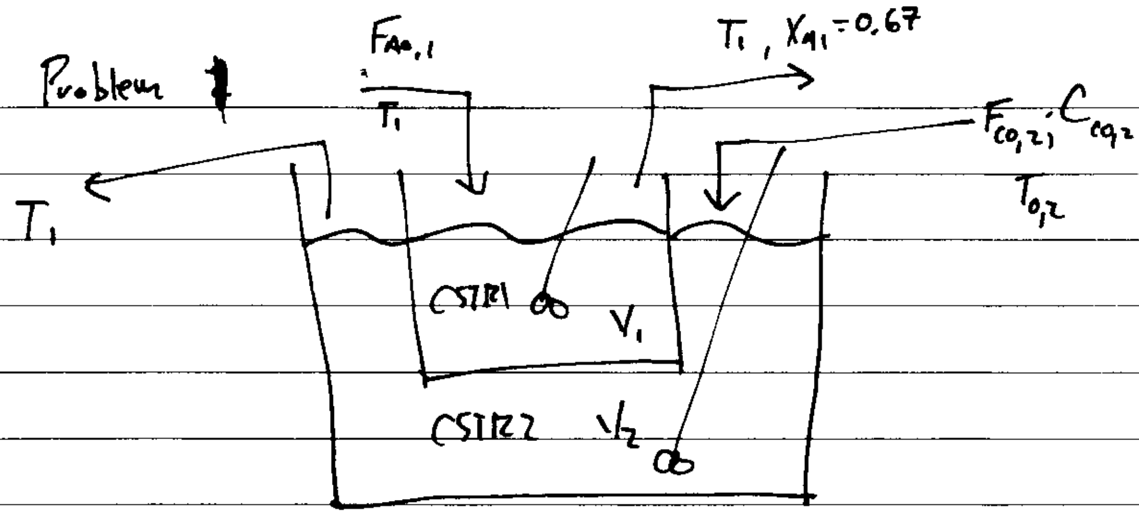
Problem



Energy Balance (total)

$$\frac{dE}{dt} = \dot{Q} + \dot{W}_S - F_{A0,1}\left(\sum_i \theta_i C_{pi}\right)(T_1 - T_1) - F_{C0,2}\left(\sum_i \theta_i C_{pi}\right)(T_1 - T_{0,2}) - F_{A0,1} X_{A1} \Delta H^\circ_{R1}$$
$$- F_{C0,2} X_{C_2} \Delta H^\circ_{R2}$$

$\rightarrow$ Steady, no shaft work, adiabatic (to surroundings), $T_1 = T_{0,2}$

$$0 = -F_{A0,1} X_{A1} \Delta H^\circ_{R1} - F_{C0,2} X_{C,2} \Delta H^\circ_{R2}$$

Mole Balance on CSTR2

$$X_C = \frac{k_2 \tau}{1 + k_2 \tau} = \frac{k_2 \left(\frac{V_2 C_{C0,2}}{F_{C0,2}}\right)}{1 + k_2 \left(\frac{V_2 C_{C0,2}}{F_{C0,2}}\right)}$$

Sub in

$$\frac{k_2 V_2 C_{C0,2}}{1 + k_2 \frac{V_2 C_{C0,2}}{F_{C0,2}}} \left(\Delta H^\circ_{R2}\right) = -F_{A0,1} X_{A1} \Delta H^\circ_{R1}$$

$$F_{C0,2} = \frac{-k_2 V_2 C_{C0,2}}{\frac{k_2 V_2 C_{C0,2} \Delta H^\circ_{R2}}{F_{A0,1} X_{A1} \Delta H^\circ_{R1}} + 1}$$

$$F_{co,2} = \frac{(-0.5\ \text{min}^{-1})(100\ L)(3\ \text{mol}\ L^{-1})}{\frac{(0.5\ \text{min}^{-1})(100\ L)(3\ \text{mol}\ L^{-1})(25000\ J\ \text{mol}^{-1})}{(50\ \text{mol}\ \text{min}^{-1})(0.67)(-50000\ J\ \text{mol}^{-1})}+1}$$

$$\boxed{F_{co,2} = 121\ \text{mol}\ \text{min}^{-1}}$$

Part b)

Energy Balance (steady, no shaft work, adiabatic to surroundings)

$$0 = -F_{co,2}C_p(T_1 - T_{0,2}) - F_{A0,1}X_{A1}\Delta H^\circ_{R1} - F_{co,2}X_{C_2}\Delta H^\circ_{R2}$$

$$0 = -F_{co,2}C_p(T_1 - T_{0,2}) - F_{A0,1}X_{A1}\Delta H^\circ_{R1} - F_{co,2}\left(\frac{k_2\frac{V_2C_{C0}}{F_{C0}}}{1+k_2\frac{V_2C_{C0}}{F_{C0}}}\right)\Delta H^\circ_{R2}$$

$$F_{A0,1}X_{A1}\Delta H^\circ_{R1} = -F_{co,2}C_p(T_1 - T_{0,2}) - F_{co,2}\left(\frac{k_2\frac{V_2C_{C0}}{F_{C0}}}{1+k_2\frac{V_2C_{C0}}{F_{C0}}}\right)\Delta H^\circ_{R2}$$

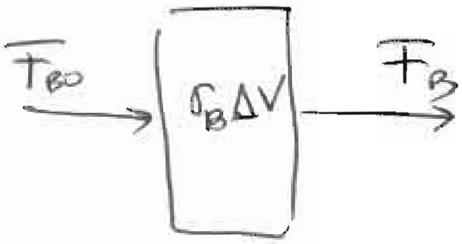
The rate of heat generated by system ① must be consumed by system ②. <u>Decreasing</u> the inlet T of system ② requires that some of the heat generated in ① be used to heat the feed to the reactor temperature (T_1). As a result, less heat is consumed by the endothermic reaction in ②, designated by the $F_{co,2}X_c$ term ∴

$$F_{co,2}X_{C_2} = \frac{k_2V_2C_{C0}}{1+\frac{k_2V_2C_{C0}}{F_{C0}}}$$

F_{C0} must <u>decrease</u>

Problem 2

(a)



$$r = K C_B^2$$

$$r_B = -2 K C_B^2$$

$$F_{B0} + r_B \Delta V - F_B = 0$$

$$F_{B0} X_B = - r_B \Delta V$$

$$C_{B0} X_B = - r_B \tau_0$$

$$\tau_0 = \frac{C_{B0} X_B}{-r_B} = \frac{C_{B0} X_B}{2 K C_B^2}$$

$$C_B = C_{B0} \frac{\overbrace{(1-X)}^{\sim 1}}{\underbrace{(1+\varepsilon X)}_{\substack{\sim 1 \\ \text{for low } X}}} \left(\frac{T_0}{T}\right) \cancelto{1}{\left(\frac{P}{P_0}\right)} = C_{B0}\left(\frac{T_0}{T}\right)$$

$$\tau_0 = \frac{\cancel{C_{B0}} X_B}{2 K(T) C_{B0}^{\cancel{2}}} \left(\frac{T}{T_0}\right)^2 = \frac{X_B \nu_0}{2 A \exp\left(-\frac{E_a}{RT}\right) C_{B0}} \left(\frac{T}{T_0}\right)^2$$

(b) If $X = 0.9$ our expression won't apply because we won't be able to assume an uniform concentration and Temperature throughout the reactor.

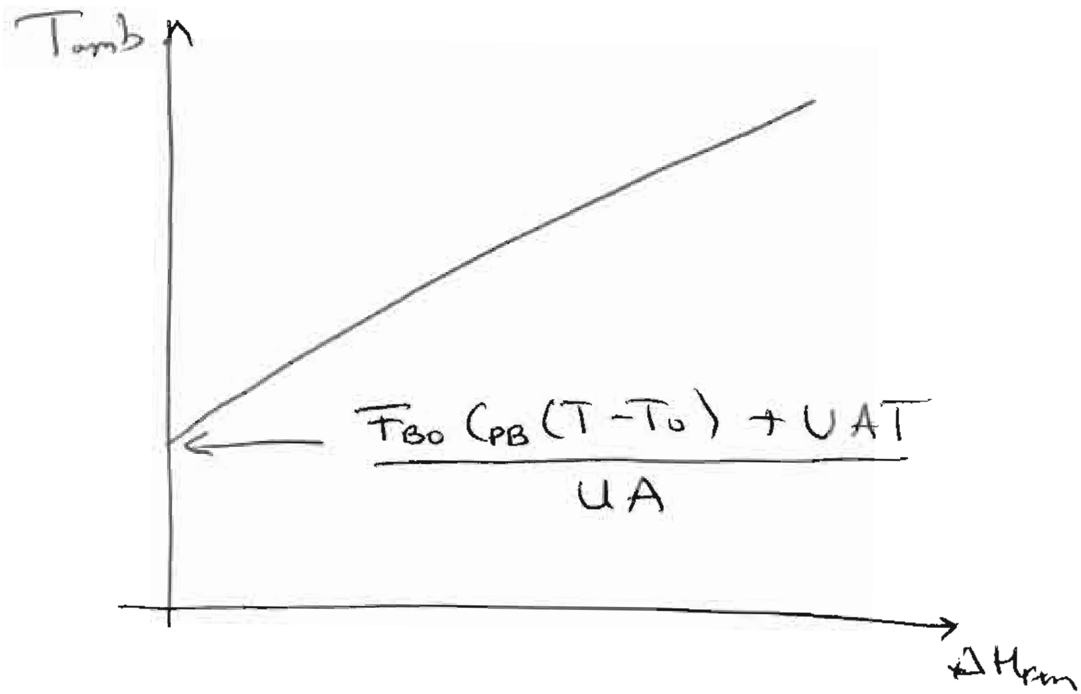
(c)

Energy Balance

$$UA(T - T_{amb}) + F_{B0} X_B \Delta H_{rxn} + F_{B0} C_{pB}(T - T_0) = 0$$

$$\Delta C_p = 0 = C_{p,C} - 2C_{p,B} \Rightarrow \Delta H_{rxn} = \Delta H_{rxn}^{\circ}$$

$$\Rightarrow T_{amb} = \frac{F_{B0} X_B \Delta H_{rxn}^{\circ} + F_{B0} C_{p,B}(T - T_0) + UAT}{UA}$$



Problem 3

$$r = \frac{r_c}{1/2} = 2 r_c = 2 k_c \frac{C_{cs}^2}{C_T}$$

$$K_B = \frac{C_{cs}}{C_{AS} \cdot P_B} \qquad C_{AS} = K_A P_A C_S$$

$$C_{cs} = K_B P_B C_{AS} = K_B K_A P_B P_A C_S$$

site balance:

$$C_T = C_S + C_{AS} + C_{cs} + C_{DS}$$

$$C_{DS} = \frac{P_D \cdot C_S}{K_D}$$

$$C_T = \underbrace{\left(1 + K_A P_A + K_B K_A P_B P_A + \frac{P_D}{K_D} \right)}_{\Gamma} C_S$$

$$C_S = \frac{C_T}{\Gamma}$$

$$C_{cs} = K_B K_A P_B P_A \frac{C_T}{\Gamma}$$

$$r = \frac{2 k_c (K_B K_A P_B P_A)^2 C_T}{(1 + K_A P_A + K_B K_A P_B P_A + P_D/K_D)^2}$$

(b) If S is MASI

$$C_T \approx C_S$$

$$C_{CS} = K_B K_A P_B P_A C_T$$

$$r = 2 k_c (K_B K_A P_B P_A)^2 C_T$$

(c) $$k_{eff} = 2 k_c K_B K_A C_T$$

$$\frac{d \ln k_{eff}}{d\, 1/T} = -\frac{E_c + \Delta H_B + \Delta H_A}{R}$$

$$E_{app} = E_c + \Delta H_B + \Delta H_A$$