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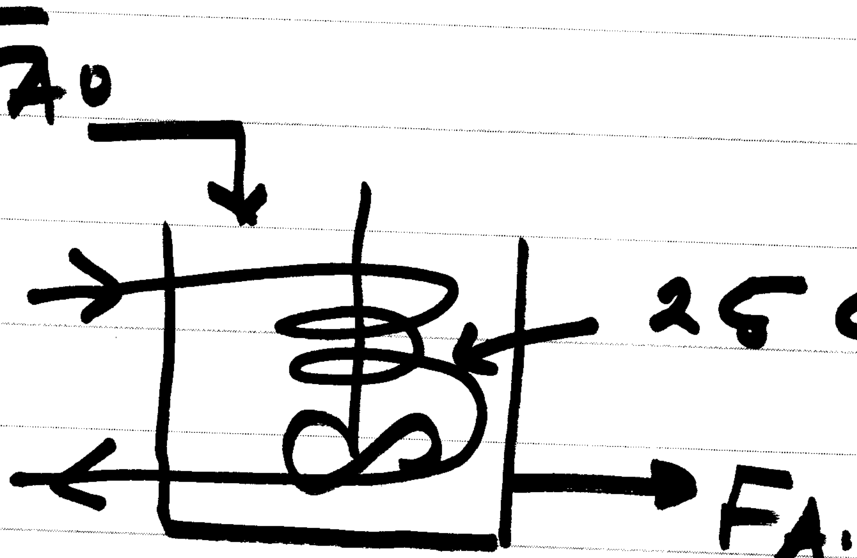
Lec. 39 (11/12/12)

Advanced Reaction Engineering

Further Considerations in Energy Balance

$$
\begin{tikzcd}
A \arrow[r, shift left] \arrow[d, shift left] & B \arrow[l, shift left] \arrow[d, shift left] \\
D \arrow[u, shift left] \arrow[r, shift left] & C \arrow[l, shift left] \arrow[u, shift left]
\end{tikzcd}
$$



All Rxns are instataneous.

$$\frac{C_B}{C_A} = K_1 \; ; \; \frac{C_C}{C_B} = K_2 \; ; \; \frac{C_D}{C_C} = K_3$$

$K_1 = 1$, $K_2 = 2$, $K_3 = 3$

$\Delta H_1 = 10 \frac{kcal}{mol}$ $\Delta H_2 = 20 \frac{kcal}{mol}$ $\Delta H_3 = 30 \frac{kcal}{mol}$

$A \rightarrow B$ X_1

$B \rightarrow C$ X_2

$C \rightarrow A$ X_3

Stoichiometric Table

$$F_A = F_{A0}(1 - X_1)$$

$$F_B = F_{A0}(X_1 - X_2) + \cancel{F_{B0}}$$

$$F_C = F_{A0}(X_2 - X_3) + \cancel{F_{C0}}$$

$$F_D = F_{A0} X_3 + \cancel{F_{D0}}$$

$$\frac{C_B}{C_A} = \frac{F_{A0}(X_1 - X_2)}{F_{A0}(1 - X_1)} = K_1 = 1$$

$$\frac{C_C}{C_B} = \frac{F_{A0}(X_2 - X_3)}{F_{A0}(X_1 - X_2)} = K_2 = 2$$

$$\frac{C_D}{C_C} = \frac{F_{A0}X_3}{F_{A0}(X_2 - X_3)} = K_3 = 3$$

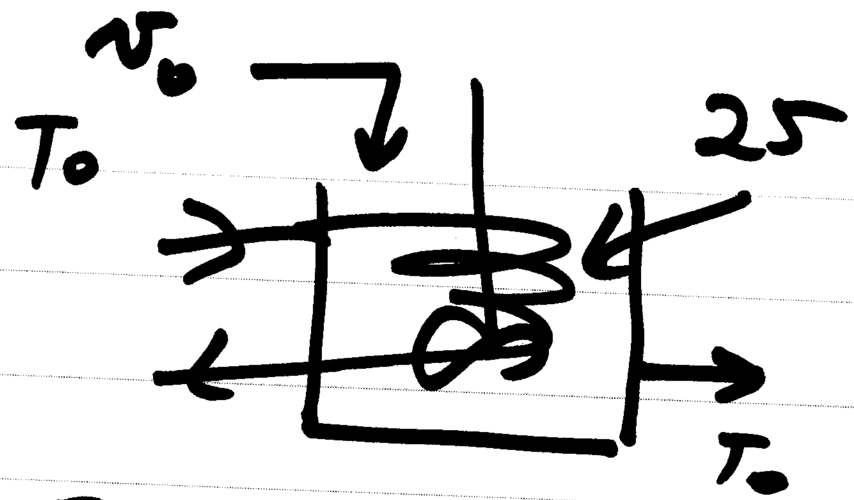
$\cancel{X_2 = X_3 = 4(1-X_1)}$

$X_1 - X_2 = 1 - X_1 \quad -(1)$

$X_2 - X_3 = 2(X_1 - X_2) \quad - (2)$

$X_3 = 3(X_2 - X_3) : (3)$

Solving $X_1 = 0.9$; $X_2 = 0.8$; $X_3 = 0.6$



$$A \rightleftharpoons B \rightleftharpoons C \rightleftharpoons D \rightarrow A$$

Energy Balance:

$$\cancel{V \hat{C}_p \frac{dT}{dt}} = \cancel{v_0 C_p (T_0 - T)} + \sum_{k=1}^{p} r_k (-\Delta H_k) V + Q - \cancel{W_s}$$

$$\sum_{k=1}^{p} r_k (-\Delta H_k) V + Q = 0$$

$$A \underset{2}{\overset{1}{\rightleftarrows}} B \rightarrow C - D - A$$

$$\sum_{k=1}^{\#\,rxns} r_k(-\Delta H_k)V + Q = 0$$

Find Q to be added or removed.

$$r_1(-\Delta H_1) + r_2(-\Delta H_2) + r_3(-\Delta H_3)$$
$$+ r_4(-\Delta H_4) + r_5(-\Delta H_5) + r_6(-\Delta H_6)$$
$$+ r_7(-\Delta H_7) + r_8(-\Delta H_8) + Q = 0$$

$$V \Delta H_1 (r_1 - r_2) + \Delta H_2 (r_3 - r_4) V$$

$$+ \Delta H_3 (r_5 - r_6) V + \Delta H_4 (r_7 - r_8) V + Q = 0$$

$$\Delta H_1 + \Delta H_2 + \Delta H_3 + \Delta H_4 = 0$$

$$\Delta H_4 = -(\Delta H_1 + \Delta H_2 + \Delta H_3)$$

$$V \Big\{ \Delta H_1 (r_1 - r_2) + \Delta H_2 (r_3 - r_4) + \Delta H_3 (r_5 - r_6)$$

$$+ (r_7 - r_8)(\Delta H_1 + \Delta H_2 + \Delta H_3) \Big\} + Q = 0$$

$F_{A0} = 1\,\text{mol}/s$

$X_1 = 0.9 \quad X_2 = 0.8 \,.\, X_3 = 0.6$

the above eqn simplifies to

$$F_{A0} X_1 (-\Delta H_1) + F_{A0} X_2 (-\Delta H_2) + F_{A0} X_3 (-\Delta H_3) + Q = 0.$$

$$\cancel{A \underset{2}{\overset{1}{\rightleftharpoons}} B \underset{4}{\overset{3}{\rightleftharpoons}} C \underset{6}{\overset{5}{\rightleftharpoons}} D \rightleftharpoons A}$$

$$\underline{\underline{A}} \underset{1}{\overset{2}{\rightleftharpoons}} B \underset{3}{\overset{4}{\rightleftharpoons}} C \underset{5}{\overset{6}{\rightleftharpoons}} D \underset{7}{\overset{8}{\rightleftharpoons}} \underline{\underline{A}}$$

Energy Balance eqn simplifies as

$$F_{A0} X_1 (-\Delta H_1) + F_{A0} X_2 (-\Delta H_2) + F_{A0} X_3 (-\Delta H_3) + Q = 0$$

$$(1)(0.9)(10) + (1)(0.8)(+20) + (1)(0.6)(30) + Q = 0.$$

$$9 + 16 + 18 + Q = 0 \Rightarrow Q = 43 \ \frac{kcal}{min.}$$

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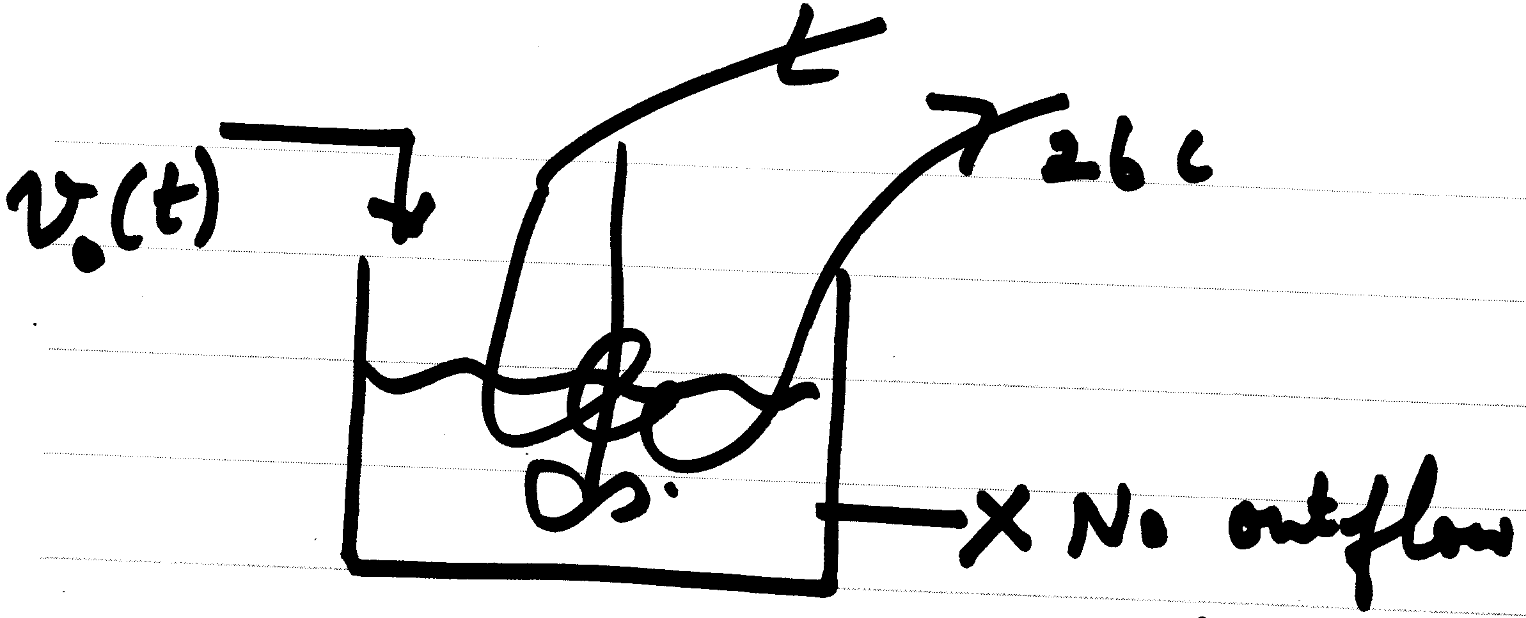


$A \to B$

$T = 38\ C$

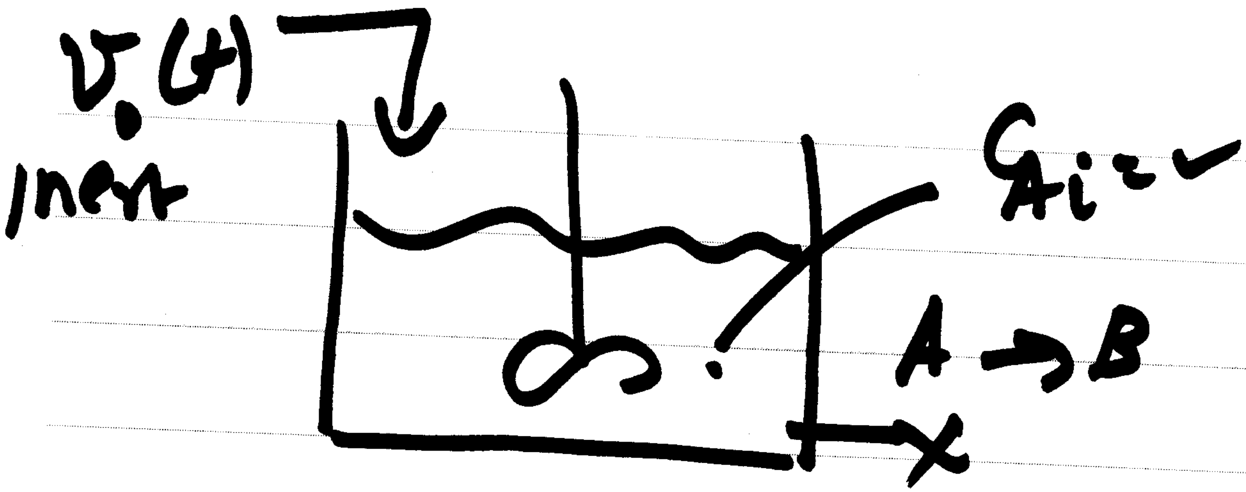
$k = 0.36/hr$

$V_i = 1.5\ M^3.$

$T_c = 26\ C$

$C_p = (0.5)(800)\ kcal/M^3 \cdot C.$

$C_{Ai} = 8\ kmol/M^3$



$$r_A = -kC_A$$

Material Balance

$$\cancel{F_{A0}} - \cancel{F_A} + r_A V = \cancel{\frac{d}{dt}N_A} \quad \frac{dN_A}{dt}$$

$$\boxed{-kC_A V = \frac{dN_A}{dt}}$$

$$\textcircled{V} C_A$$

$$-k(C_A V) = \frac{d}{dt} N_A.$$

$$(C_A V) = N_A.$$

$$V = (V_i + v_0 t)$$

$$-kN_A = \frac{dN_A}{dt}$$

$$\boxed{N_A = N_{A0} \exp(-kt)}$$

$$V \cancel{C_p} \frac{dT}{dt} = v_0 C_p (T_0 - T) + \sum r_k (\Delta H_k) V + Q - \cancel{W_S}$$

$$v_0(t)\, C_p (T_0 - T) + r_1 (-\Delta H^*) V + Q$$

$$r_1 = k C_A$$

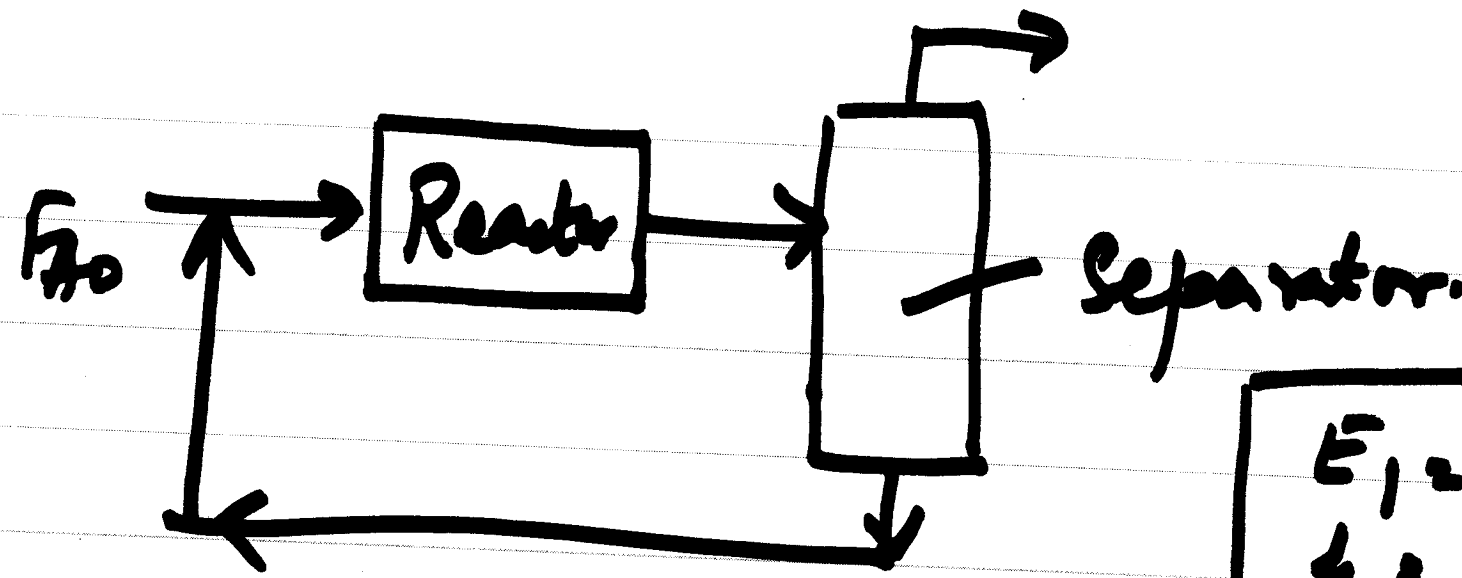
$$v_0(t)\, C_p (T_0 - T) + k C_A (-\Delta H_1^*) V + Q$$

$$0 = v_0(t)\,C_p\,(T_0 - T) + (k N_A)(-\Delta H_1^*) + \cancel{\dot{Q}}$$

$$0 = v_0(t)(400)(-82) + k N_A \exp(-kt)(\Delta H_1^*) \downarrow + \cancel{\dot{Q}}$$

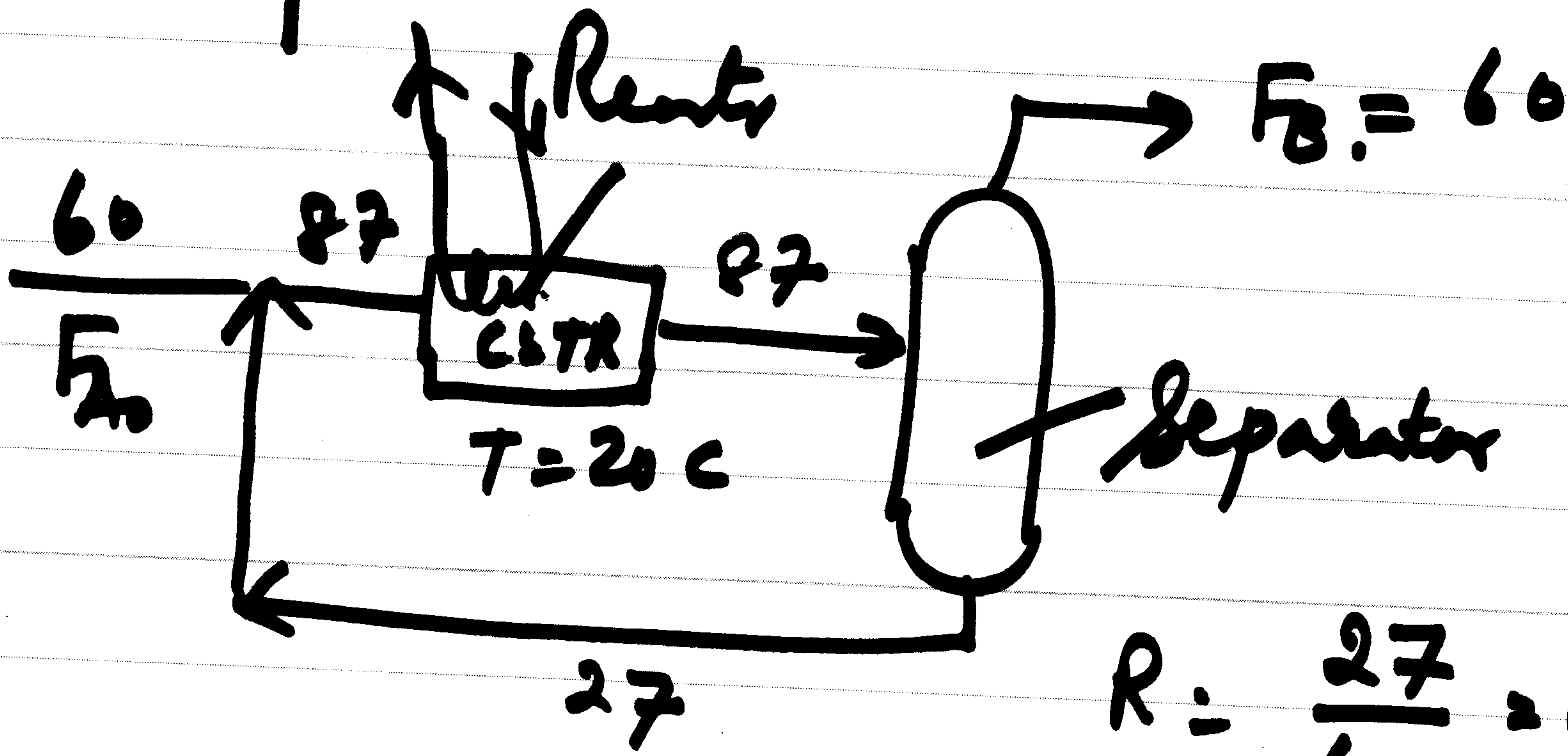
$$0 = -v_0(t)\{4800) + k\; 12 \exp(-kt)\left(20{,}000 \frac{kcal}{m}\right) + \cancel{\dot{Q}}$$

$$v_0(t) = f(\,)$$



$E_1 = 20$ kcal/mol
$k_1 = 0.4$/min at 20C
$k_2 = 0.1$/min at 20C

F_{A0} = Pure A
Production – ~~..~~ 60 mol/min
Feed = 49 C
Molar density = 20 mol/~~...~~ lit
C_p = 1.0 kcal/L·C
h = 5 kcal/M^2·min·C.
T_c = 5 C



$$R = \frac{27}{60} = 0.45.$$

Q. What is the best temperature of operation $A \underset{2}{\overset{1}{\rightleftharpoons}} B$ $E_2 = ?$

$$r_B = k_2 C_B - k_1 C_A = k_2 C_{A0}(1-x) - k_1 C_{A0} x$$

$$\left(\frac{\partial r_B}{\partial T}\right)_x = 0 \quad : \quad \frac{x_m}{1-x_m} = \frac{k_1}{k_2}\left(\frac{E_1}{E_2}\right).$$

$$\frac{x_m}{1-x_m} = \frac{0.4}{0.1}\left(\underline{20}\right) = 80$$

$$E_1 - E_2 = \Delta H$$

$$E_2 = E_1 - \Delta H.$$

$$\left(\frac{\partial r}{\partial T}\right)_x = 0 = \frac{X_m}{1 - X_m} = K \frac{E_1}{E_2}$$

$$\overset{20c}{=} (4)\frac{(25)}{(45)} = 2.2$$

$$\frac{X_m}{1 - X_m} = 2.2.$$

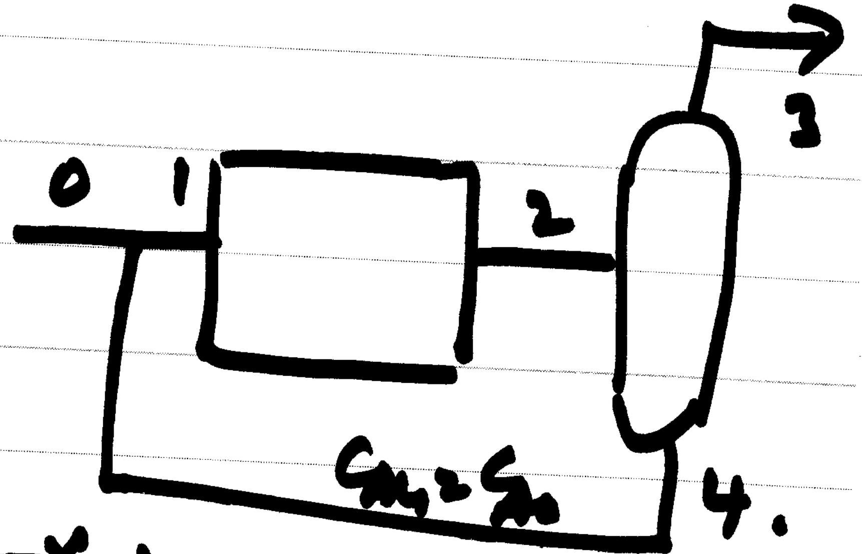
$$3.2 X_m = 2.2$$

$$X_2 = X_m = 2.2/3.2 = \underline{\underline{0.687}}.$$

$$F_{A1} - F_{A2} + r_{A2} V = 0.$$

$$T = 20\ C$$

$$X_m = 0.667.$$



$$F_{A1} - F_{A1}(1-X_2) + \left[-k_1 C_{A1}(1-X_2) + k_2 C_{A1} X_2\right] V = 0.$$

$$F_{A1} X_2 - \left[k_1 C_{A1}(1-X_2) + k_2 C_{A1} X_2\right] V = 0$$

$$F_{A1} x_2 - k_1 C_A (1 - x_2) V$$

$$+ k_2 C_A x_2 V = 0 \qquad \underline{\underline{T = 20 C}}$$

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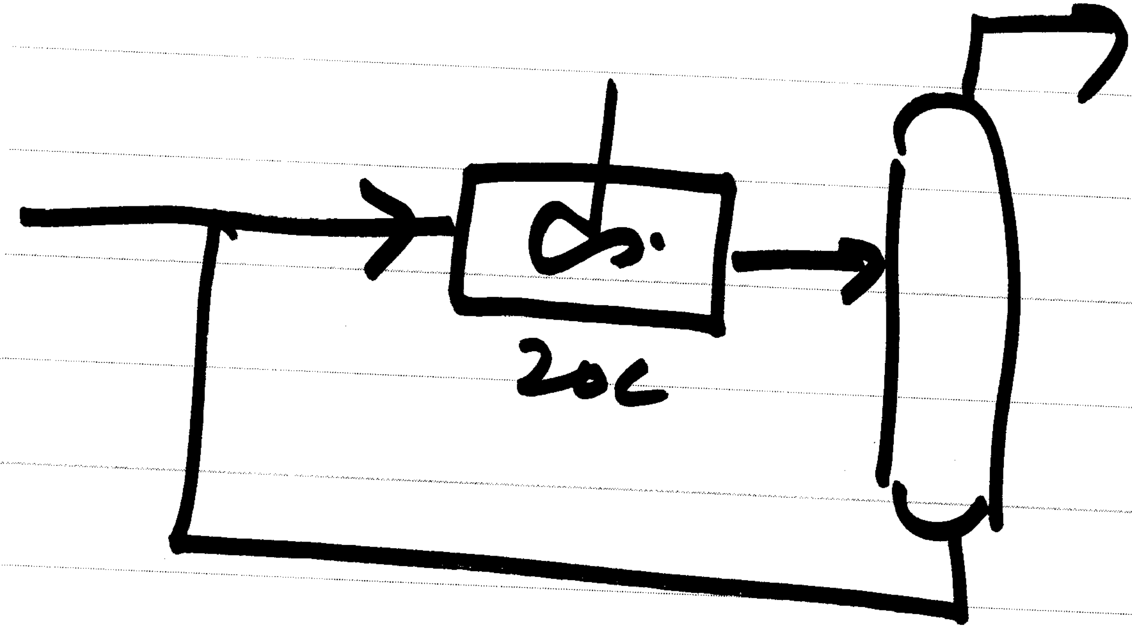
$$F_{A1} = F_{A0} + F_{A4}$$

$$= F_{A0} + F_{A2}$$ defined w.r.t part 1.

$$= F_{A0} + F_{A1}(1 - X_2)$$

$$F_{A1} X_2 = F_{A0}$$

$$F_{A1} = (F_{A0}/X_2) = \frac{60 \text{ mol}/\text{min}}{0.687} = 87 \frac{\text{mol}}{\text{min}}$$



$$V C_p \cancel{\frac{dT_i}{dt}} = v_0 (T_i - T) C_p + \sum_{i=1}^{\#rxn} r_i (-\Delta H_i) V + Q - \cancel{W_s}$$

$$0 = 3\frac{lt}{min}(40-20)\,10 + (r_1 - r_2)(20)V + Q =$$

$$F_{A1} - F_{A1}(1 - X_2) + (r_2 - r_1)V = 0$$

$$+ F_{A1}X_2 + (r_2 - r_1)V = 0$$

$$F_{A1}X_2 = (r_1 - r_2)V = F_{A0}$$

$$= 60 \text{ mol/min}$$

$$0 = (3)(40 - 20)(1.0) + (F_{A0})(20) + Q.$$

$$Q = -1140 \text{ kcal/min}$$

$Q = -1140 \text{ kcal/min}$

$T = 20 \, C$

$T_C = 5 \, C$

$Q = U A \Delta T.$

$(5 \text{ kcal/m}^2 \cdot \text{min } C)(A)(20-5) = 1140$

$$A = \frac{1140}{(5)(15)} = 15.2 \, M^2$$