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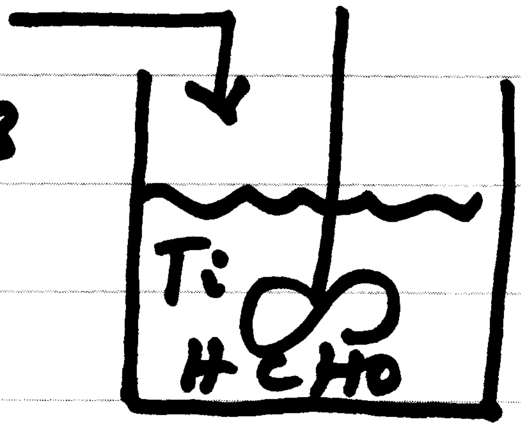
Advanced Chemical Reaction Engineering

Practice Problems - Energy Balance in Stirred Vessels

23 Nov 2012
1100 - [illegible]

Semi batch operation of a stirred vessel.

$v_0 = 10\,L/min$
NH_3 (A)
C_{A0}
$T_{A0} = 0$



(B)

$4NH_3 + 6HCHO = N_4(CH_2)_6 + 6H_2O$
(A)

Reaction in instantaneous

$V_i = 2000$ Lit

$C_{Bi} = 15$ gmol/L

$C_p = 1000$ Cal/L.c for mixture

$C_{A0} = 15$ gmol/L

$\Delta H = -74$ kcal/mol. HMT.

$T_i = 0$ c

(1) How long does it take for HCHO to be completely consumed

(2) If process is adiabatic how long does it take to reach 60 c

(3) If reaction mixture is to be maintained at 60°c how much heat is to be added or removed.

$$(V)(r_A) = (-r_1 V)(-4) = F_{A0} = 10\,\frac{L}{min} \times 15\,\frac{gm}{L}$$

$$4\,NH_3 + 6\,HCHO = N_4(CH_2)_6 + 6\,H_2O$$

$$r_1 V = 150/4 = 37.5\ gm/mi$$

Balance B

$$\cancel{F_{B0}} - \cancel{F_{B0}} + r_B V = \frac{d}{dt} N_B$$

$$(-r_1)(6)V = \frac{d}{dt} N_B$$

$$t = \frac{N_{Bi}}{(37.5)6} = \frac{15 \times 2000}{6 \times 37.5} = 133\ min$$

$$\sum N_i \frac{dH_i}{dt} = \sum_{i=1}^{nspecies} F_{io} (H_{io} - H_i) + \sum_{i=1}^{prxn} r_i V (-\Delta H^*) + \cancel{Q} - \cancel{W_s}$$

$$V C_p \frac{dT}{dt} = v_o \tilde{C}_p (T_o - T) + r_1 V (-\Delta H^*).$$

exo

$$(V_i + v_o t) \frac{dT}{dt} = (10)(10)(0 - T) + (37.5)(+74.6)$$

$$(2000 + 10t) \frac{dT}{dt} = -10T + (37.5 \times 74.6)$$

$$= -10T + 2797.5$$

$$\frac{dT}{dt} + \frac{T}{200 + 10t} = \frac{2797}{200+t}$$

after integration

$$T(200+t) = (279.7)\,t$$

↑

$61^\circ C$

what is t ⇒

$$t = \frac{12000}{219.7} = 54.6 \text{ min.}$$

Mole bal: T = 60 C

Energy Balance

$v_0 C_p (T_0 - T) + r_1 V (-\Delta H_1^*) + Q - \cancel{W_s}$

$= \cancel{V C_p \frac{dT}{dt}}$

$(10)(1.0)(0 - 60) + (37.5)(74.6) + Q$.

$Q = -2197$ kcal/min. [heat has to be removed.]

$A \rightarrow B;\ A \rightarrow C$

$T = 54.5°$

$v_0 = 0.0566\ m^3/s$

$\rho = 72\ kg/m^3$

$c_p = 0.8\ kcal/kg\ C$

$C_{A0} = 15\ mol/L$

$V = 1.0\ m^3$

$h = 0.55\ kcal/m^2 . C . s$

Heating Medium: Sat Steam at 100 C

$A_1 = (3)10^8/s$

$A_2 = (2)10^{14}/s$

$E_1 = 15000\ cal/mol.$

$E_2 = 25000\ cal/mol$

$\Delta H_1 = -9000\ cal/mol$

$\Delta H_2 = 1388\ cal/mol.$

(1) Show that T which maximum production of B

$$k_2 \tau = E_1 / (E_2 - E_1)$$

(2) Find Conversion, Reactor Temp.

(3) What is area of Cooling / heating coil required.

Stoichiometric Table

A	$F_{A0}(1 - X_1 - X_2)$	$A \rightarrow B$
B	$F_{A0} X_1 + \cancel{F_{B0}}$	
C	$F_{A0} X_2 + \cancel{F_{C0}}$	

$$C_A = \frac{F_A}{v} = \frac{F_{A0}(1 - X_1 - X_2)}{v_0}$$

$$= C_{A0}(1 - X_1 - X_2)$$

Material Balance for B

$$0 - F_B + r_B V = 0$$

$$0 - F_{A0} X_1 + k_1 C_{A0}(1 - X_1 - X_2) V \quad -V\,/$$

A → C

Material Balance for Comp C

$0 = F_{A0} X_2 + k_2 C_{A0} (1 - X_1 - X_2) V$ — (2)

From (1) and (2)

$$\frac{X_1}{X_2} = \frac{k_1}{k_2} \quad — \quad (3).$$

Putting eq(3) in eqn (1)

$-F_{A0} X_1 + k_1 C_{A0} \left(1 - X_1 - \frac{k_2}{k_1} X_1\right) V$

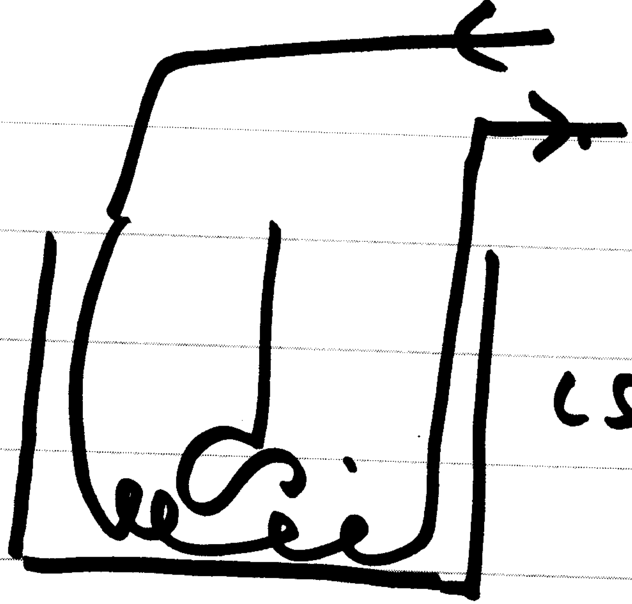
$$X_1 \left(1 + k_1 \tau + k_2 \tau \right) = k_1 \tau$$

$$X_1 = \frac{k_1 \tau}{1 + k_1 \tau + k_2 \tau}$$

Maximise X_1 (w.r.t) T.

$$\left(\frac{dX_1}{dT}\right) = \frac{(k_1 E_1 / RT^2)\, \tau}{(1 + k_1 \tau + k_2 \tau)} - \frac{k_1 \tau \left[\frac{k_1 E_1}{RT^2} \tau + \frac{k_2 E_2}{RT^2} \tau \right]}{(1 + k_1 \tau + k_2 \tau)^2}$$

$$= 0$$



$A \rightarrow B \qquad r_1 = k_1 C_A$ (Desired)

$A \rightarrow C \qquad r_2 = k_2 C_A.$ (undesired)

15

$E_1 = 15000$ cal/mol

$E_2 = 25000$ cal/mol

$$(k_2 \tau) \text{ for Max B} = \frac{15000}{25000 - 15000} = 1.5$$

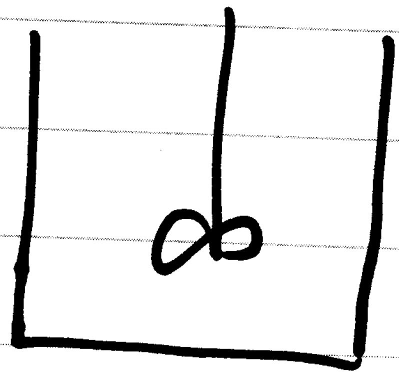
$$\tau = \frac{V_R}{v_0} = \frac{(1.0)}{0.066} = \underline{\underline{15.1 \text{ s}}}$$

$$(k_2)\,\tau = 1.5$$

$$k_2 = 1.5/\tau = 1.5/15.1 = 0.1/\text{s}$$

$$E_1 (1 + k_2 \tau) = k_2 E_2 \tau$$

$$k_2 \tau = \frac{E_1}{E_1 - E_2}$$



$A \rightarrow B$

$A \rightarrow C$

1b

$$k_2 = A_2 e^{-E_2/RT}$$

$$0.1 = (2)10^{14} e^{-25000/1.987(T)}$$

Solve for T = 83.5 C (Accuracy of Calculation is important).

k_1 (83.5)

$$= (3)10^{8}\left(\exp\left(\frac{-15000}{(1.987)(357)}\right)\right).$$

$= 0.197/s$

$$x_1 = \frac{k_1 \tau}{1 + k_1 \tau + k_2 \tau}$$

$$= \frac{(0.197)(15.1)}{1 + (0.197)(15.1) + (0.1)(15.1)}$$

$$x_1 = 0.542$$

$$x_2 = \frac{k_2}{k_1} x_1 = (0.542)\left(\frac{0.1}{0.197}\right) = 0.273$$

$$\sum N_i \frac{dH_i}{dT} =$$

$$\sum F_{i0} (H_{i0} - H_i)$$

$$+ \sum_{i=1}^{p_{rxn}} r_i (-\Delta H_i^{*}) V + \dot{Q} - \dot{W}_s$$

$$H_i = H_i^{\circ}(T_R) + C_{pi} (T - T_R)$$

$$0 = v_0 \hat{C}_p (T_0 - T)$$

$$+ \underbrace{r_1 V}_{F_{A0} x_1} (-\Delta H_1^R) + \underbrace{r_2 V}_{F_{A0} x_2} (-\Delta H_2^R) + Q.$$

$$0 = (0.086)(720)(0.8)(54.5 - 83.5)$$

$$+ (0.086)(15)(0.54)(9070)$$

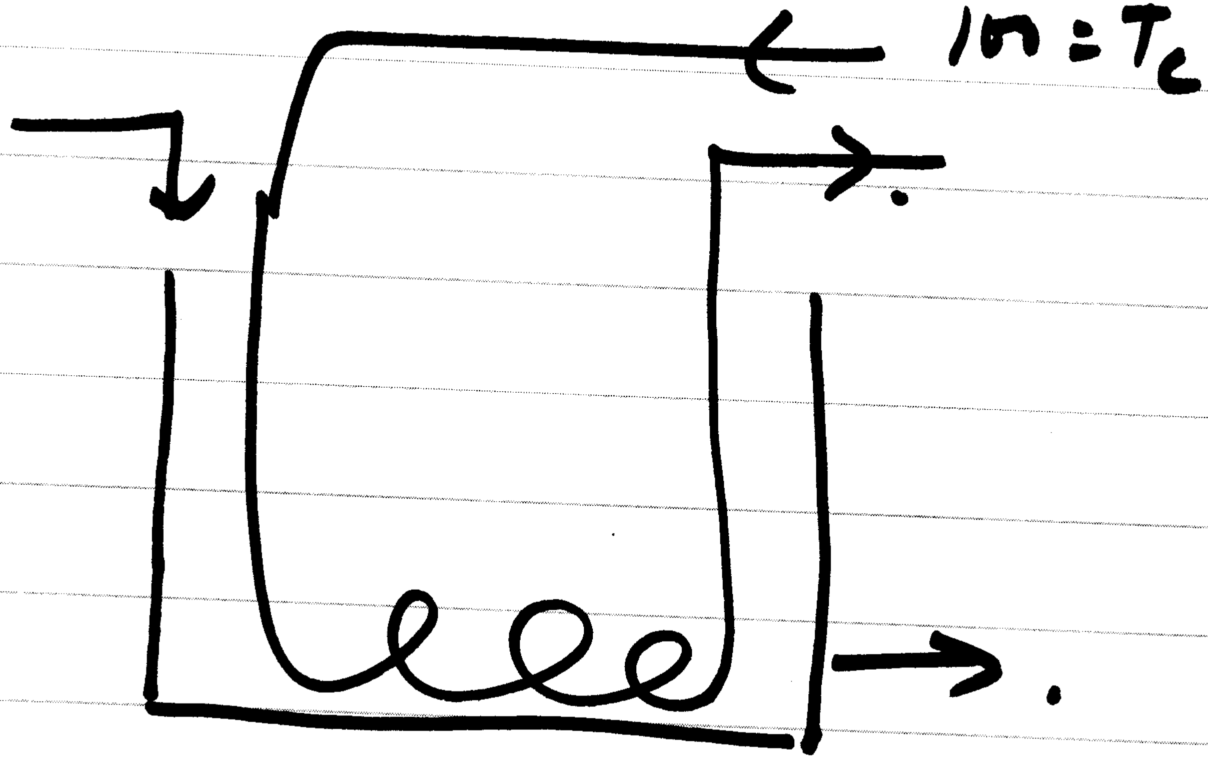
$$+ (0.086)(15)(0.22)(-13800) + Q$$

$$Q = +13 \text{ kcal/s}$$

$$Q = hA(T_c - T)$$

$$13 = (0.55)(A)(100 - 84)$$

$$A = 1.5\ m^2$$


100 = T_c