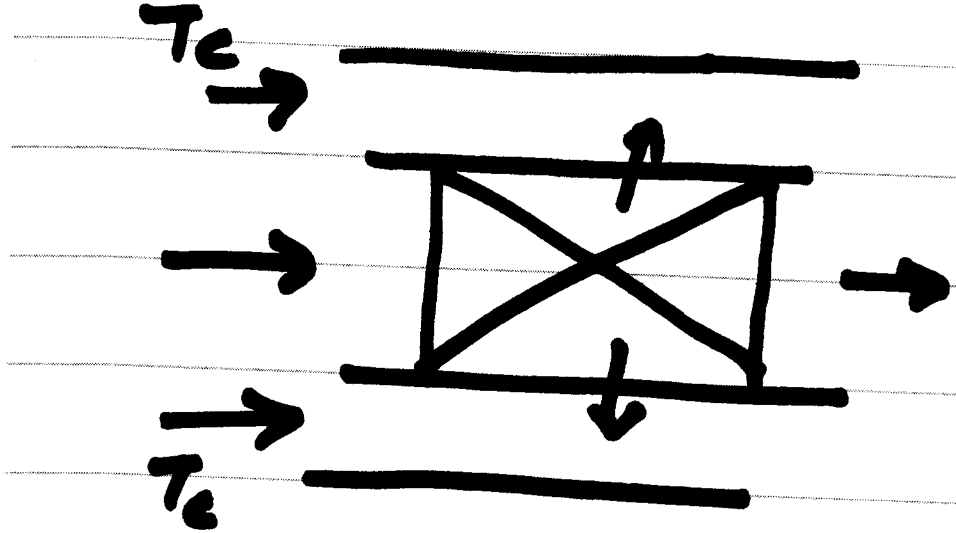
Prof. Shankar

Lec. 34 05/12/2012

Wednesday
5 Dec 2012
1030–1130

Advanced Reaction Engineering

Further Considerations in Energy Balance



k at 513 K = 1800/hr

$E = 20{,}000$ cal/mol

$\Delta H = -152$ kcal/mol

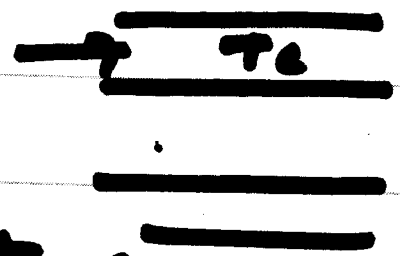
$h = 20$ kcal/m^2 hr C

$r = k C_H$.

$T_c = 25$ C

Energy Balance

$$v C_p \frac{dT}{dV} = r_1 (-\Delta H_r^*) + \frac{4h}{D}(T_c - T)$$



v - volumetric flow m^3/hr

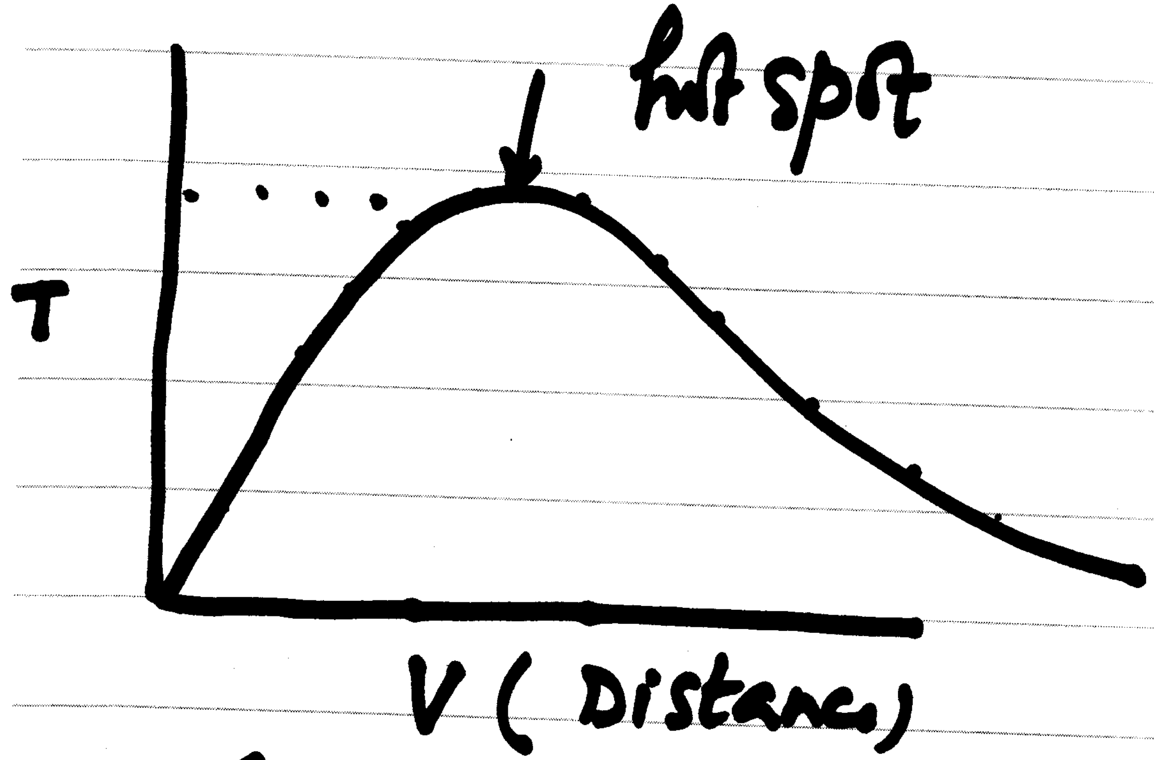
C_p = vol. sp. heat kcal/liter C

r_1 = rate function kC_H mol/L.hr

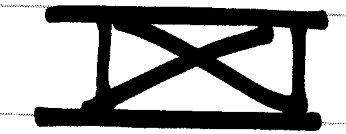
h - heat transfer coefficient kcal/m^2 hr C

D - pipe diameter m

T_c - Coolant Temp C



Wall Cooled Reactor



$$\nu C_p \frac{dT}{dV} = r_1(-\Delta H^*) + \frac{4h(T_c - T)}{D}$$

heat gen

(heat Removal)

↑ hot spot

At hot spot we have

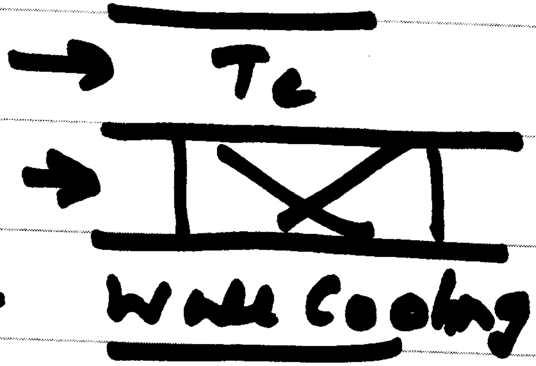
$$0 = r_1(-\Delta H_r^*) + \frac{4h}{D}(T_c - T).$$

$$\underbrace{\frac{4h}{D}(T - T_c)}_{\text{heat removal}} = \underbrace{r_1(-\Delta H_r^*)}_{\text{heat generation}} \quad \text{at hot spot.}$$

$P_t = 1$ atm

$y_{A0} = 0.1$ (HCl)

$T_0 = 140$ C



$C_2H_2 + HCl(g) = C_2H_3Cl$ (VCl)

dp (m)	T (hot spot)	X_{expt}	y_{A0}
0.05	240	0.43	0.1
0.075	240	0.39	0.1
0.125	300	0.61	0.2

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At the hot spot

$$r_1(-\Delta H_1^*) = \frac{4h}{D}(T - T_c)$$

$$r_1 = k C_H = k C_{H0}(1 - x)$$

$$k_1 C_{H0}(1 - x)(-\Delta H_1^*) = \frac{4h}{D}(T - T_c)$$

$$1 - x = \frac{4h(T - T_c)}{D k C_{H0}(-\Delta H_1^*)}$$

D	T	X
0.05	240	0.43

$$C_{A0} = \frac{P(0.1)}{(RT)} = (2.34)10^{-3} \ \frac{mol}{L}$$

$$1-X = \frac{(4)(20)(240-25)}{(0.05)(1800)(2.34)10^{-3}(152000)}$$

$$1-X = 0.537 \Rightarrow X = 0.46$$

$$1 - X = \frac{4h\,(T - T_a)}{D\,k\,C_{A0}\,(-\Delta H_1^{x})}$$

$$= \frac{(4)(20)(240 - 25)}{(0.075)(1800)(0.0047)(152000)}$$

$C_{A0} = 0.0047 \ \frac{mol}{L}$

$$1 - X = 0.178 \implies X = 0.82$$

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$$1 - X = \frac{4h(T - T_c)}{D\,k\,C_{A0}(-\Delta H_x)}$$

$$= \frac{(4)(20)(300 - 25)}{(0.025)(7.76)(1800)(1.05)10^{-3}}$$

$k(300\ C) = 7.76$

$k(240\ C)$

$C_{A0}(300\ K)$

$= (1.05)10^{-3}\ \frac{mol}{L}$

$$1 - X = 0.394$$

$$X = 0.60$$

hot spot

M d_p	X_{expt}	X_{Model}	T
.05	0.43	✓0.46	240
0.075	0.79 ✓	0.82	240
0.025	0.61	0.60	300

k_o = 1800/hr

Endothermic Reaction.

Processing at 20 mol/hr.

Heat of rxn: 20 kcal/mol.

Heat ~~balance~~ supply: 400 kcal/hr

$k = 1800/hr$

Heat transfer design

20 heat/hr

Heat:

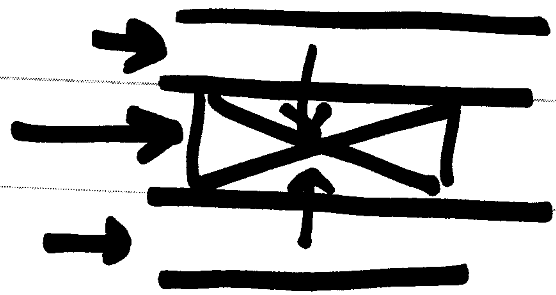
Rxn proceeds at the rate at which heat is supplied.

Endothermic Reaction
which is instantaneous

$k_1 \quad k_2$ $\qquad A \underset{2}{\overset{1}{\rightleftarrows}} B$

RXN is essentially at equilibrium

$(X)_{eq} = K/(K+1) \qquad K(T)$



Instantaneous

$$A \underset{1}{\overset{2}{\rightleftarrows}} D$$

$$v \hat{C}_p \frac{dT}{dV} = r_1(-\Delta H_1^*) + r_2(-\Delta H_2^*) + \frac{4h}{D}(T_c - T)$$

$$= \underline{\underline{(r_1 - r_2)}}(-\Delta H^*) + \frac{4h}{D}(T_c - T)$$

$$\frac{dF_A}{dV} = (r_2 - r_1)$$

$$F_{A0} \frac{dx}{dV} = (r_1 - r_2)$$

$$\frac{dx}{dV} = \frac{dx}{dT} \cdot \frac{dT}{dV}$$

$$X = \frac{K}{K+1}$$

Reactions at instantaneous so are at equilibrium.

$$\frac{dx}{dT} = \left(\frac{1}{K+1} - \frac{K}{(K+1)^2}\right)\frac{dK}{dT} \cdot \frac{1}{(K+1)^2}\left(\frac{\Delta H}{RT^2}\right)$$

Vant Hoff's Eqn

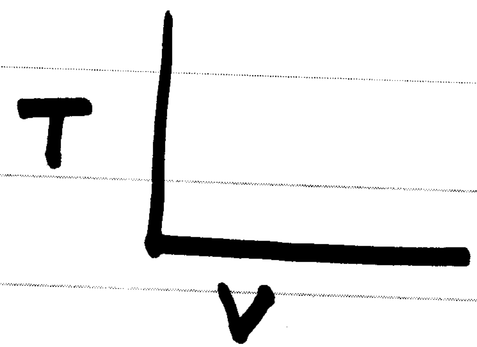
$$\frac{d\ln K}{dT} = \frac{\Delta H}{RT^2}$$

$$\left(K/K+1\right) = X$$

$$\frac{dK}{dT} = K.\left(\frac{\Delta H}{RT^2}\right)$$

$$v C_p \frac{dT}{dV} = (-\Delta H^*) F_{A0} \frac{dx}{dV} + \frac{4h}{D}(T_c - T).$$

$$v C_p \frac{dT}{dV} = (-\Delta H^*) F_{A0} \left(\frac{dx}{dT}\right) \cdot \frac{dT}{dV} + \frac{4h}{D}(T_c - T)$$

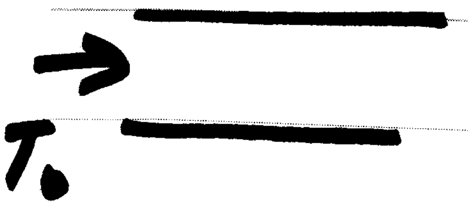


$$v C_p \frac{dT}{dV} = (-\Delta H_1^*) F_{A0} \frac{(\Delta H_1^*)}{R T^2 (K_e+1)^2} \frac{dT}{dV} + \frac{4h}{D}(T_c - T).$$

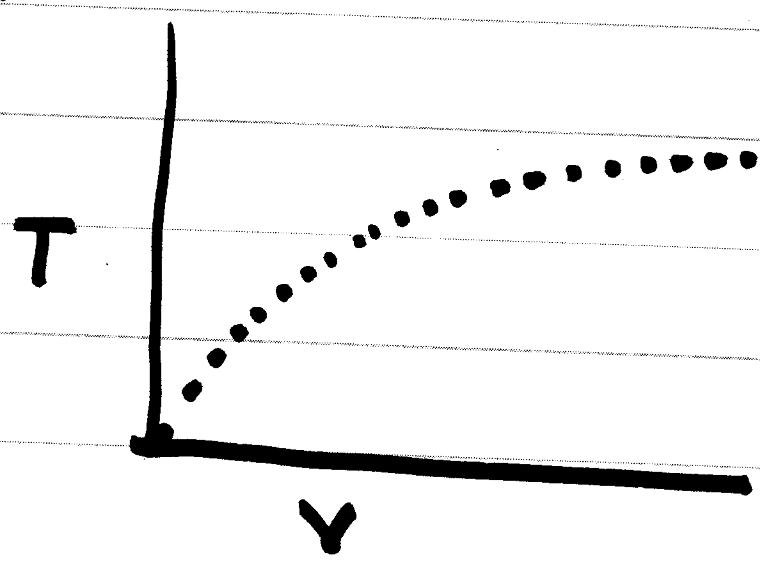
$$\frac{dT}{dV}\left\{ v C_p + \frac{(\Delta H_1^*)^2 F_{A0}}{R T^2 (K+1)^2} \right\} = \left[\frac{4h}{D}(T_c - T) \right]$$

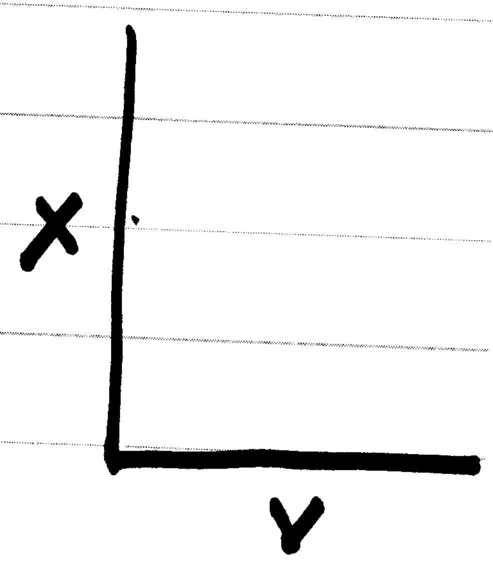
$$= f(T).$$

$$\frac{dT}{dy} = \frac{\frac{4h}{D}(T_c - T)}{\left[\nu C_p + (\Delta H_1^*)^2 F_{A0} / RT^2 (K+1)^2 \right]}$$



$$X = \left(\frac{K}{K+1}\right)$$





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① Instantaneous Rxn

$$X = \frac{K}{K+1}$$

② Reaction k : 1800/hr

Endothermic

heat transfer Rate Control : 10/hr