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Lec. 30 23/11/2012

Advanced Reaction Engineering

Practice Problems – Tubular Reactors

23 Nov 2012
Friday 1515–1615

$SO_2 + \frac{1}{2} O_2 = SO_3$

$N_2 + H_2 = NH_3$

exothermic

Reversible

Catalytic

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

$$r_B = k_1 C_A - k_2 C_B$$

$$= k_1 C_{A0}(1-x) - k_2 C_{A0}\, x \qquad (C_{B0}=0).$$

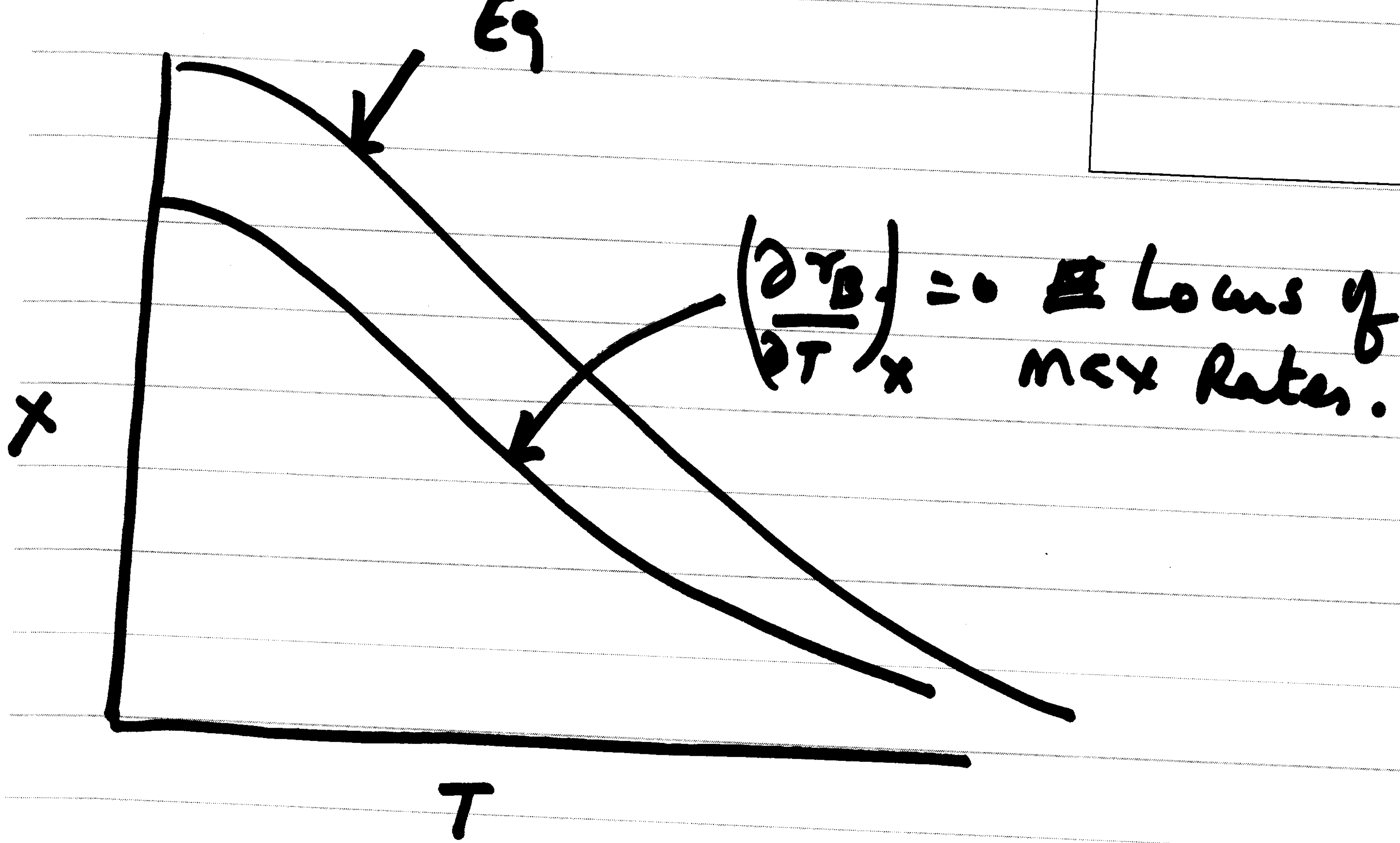
$$\left(\frac{\partial r_B}{\partial T}\right)_x = \frac{k_1 E_1}{RT^2} C_{A0}(1-x) - \frac{k_2 E_2}{RT^2} C_{A0}\, x = 0.$$

$$\left(\frac{x_m}{1-x_m}\right) = \left(\frac{k_1}{k_2}\right) \frac{E_1}{E_2} = K \frac{E_1}{E_2}$$

$$\left(\frac{\partial r_B}{\partial T}\right)_X = 0 \Rightarrow \frac{X_m}{1-X_m} = K \frac{E_1}{E_2}$$

At Eq $r_B = 0$ $\quad k_1 C_{A0}(1-X) - k_2 C_{A0} X = 0$

at Eq $\dfrac{X_e}{(1-X_e)} = \dfrac{k_1}{k_2} = K.$


Eq
$\left(\frac{\partial r_B}{\partial T}\right)_X = 0$ Locus of max Rates.
X
T

b

Tubular Reactor

Mate Balance

$$F_{A0}\frac{dx}{dV} = (r_1 - r_2) \quad - (2)$$

as adiabatic

$$v C_p \frac{dT}{dV} = (r_1 - r_2)(-\Delta H_1^*) + \cancel{Q} - \cancel{W_s} \quad - (1)$$

$(1/2)$

$$\frac{v C_p}{F_{A0}}\frac{dT}{dx} = -(\Delta H_1^*)$$

$A \rightleftarrows B$

Tubular Reactor

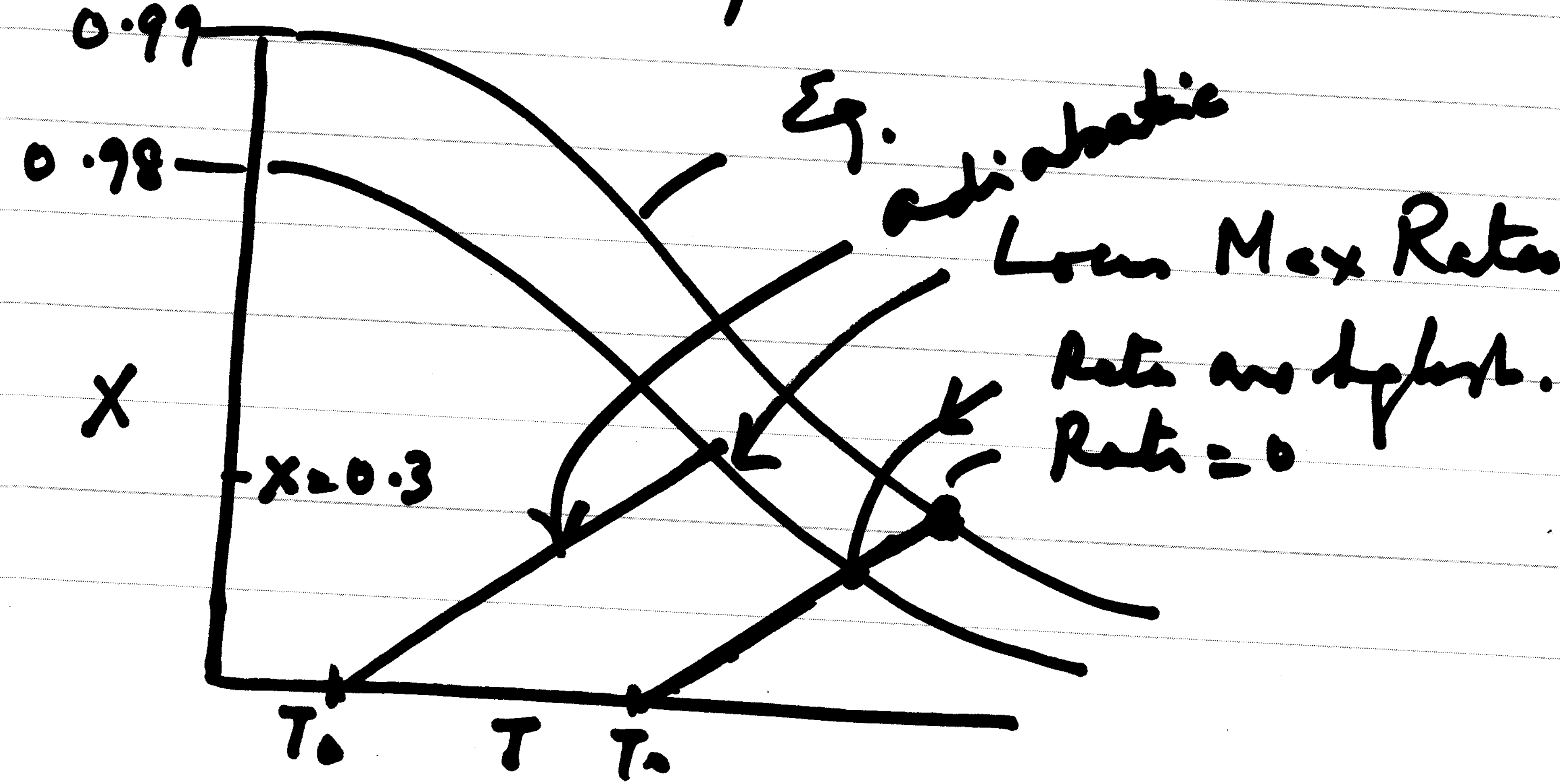
$$\frac{v\,C_p}{F_{A0}}\frac{dT}{dx} = -(\Delta H_1^*)$$

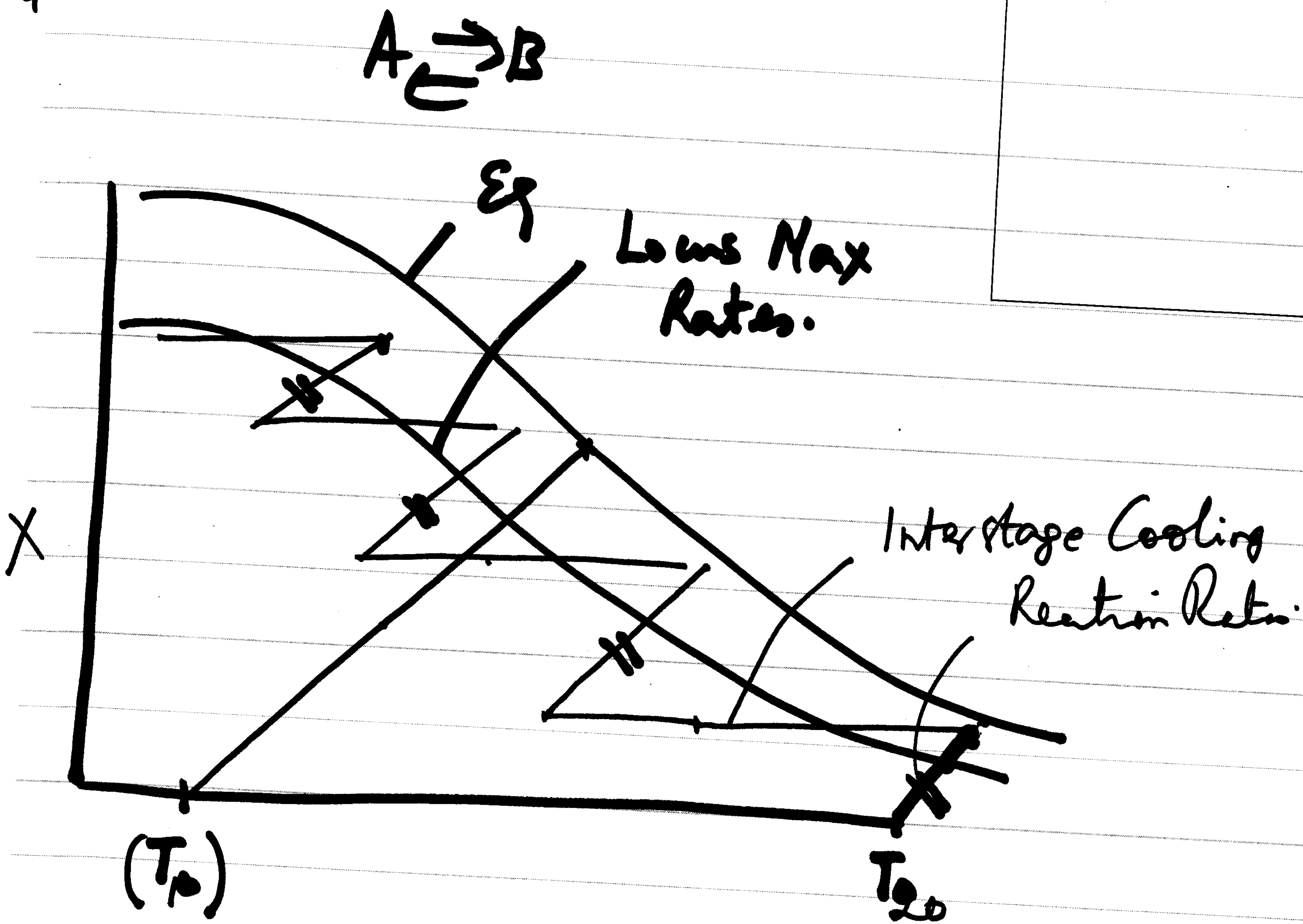
$v : v_0$

$$\frac{\cancel{v_0}\,C_p}{\cancel{v_0}\,C_{A0}}\frac{dT}{dx} = (-\Delta H_1^*)$$

$$\frac{dT}{dx} = (C_{A0})\left(-\frac{\Delta H_1^*}{C_p}\right)$$

$$\frac{dT}{dx} = C_{A0}\left(\frac{-\Delta H^*}{C_p}\right)$$




A ⇌ B
Eq
Locus Max Rates.
Interstage Cooling
Reaction Rates
X
(T_p)
T_20

$C_{A0} = 1.6$ mol/L

$C_p = 1.0$ cal/kg·C

$T_0 = 21$

$v_0 = 5\ m^3/hr$

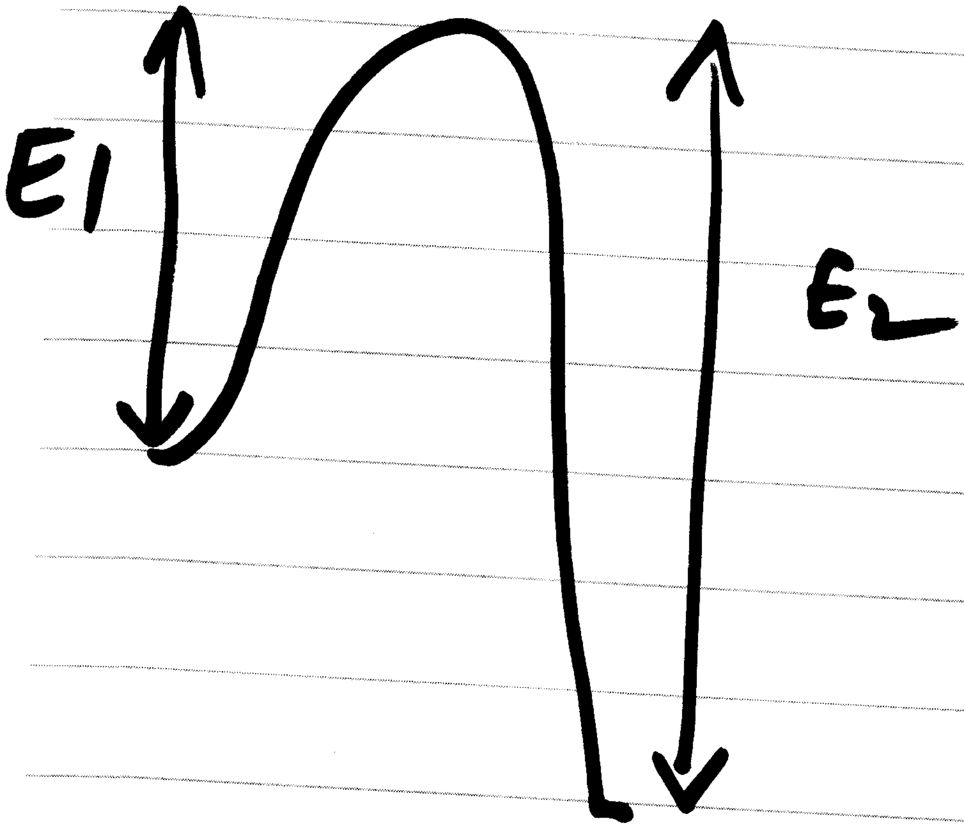
$\rho = 0.9$ g/mL

$E_1 = 2500$ cal/mol

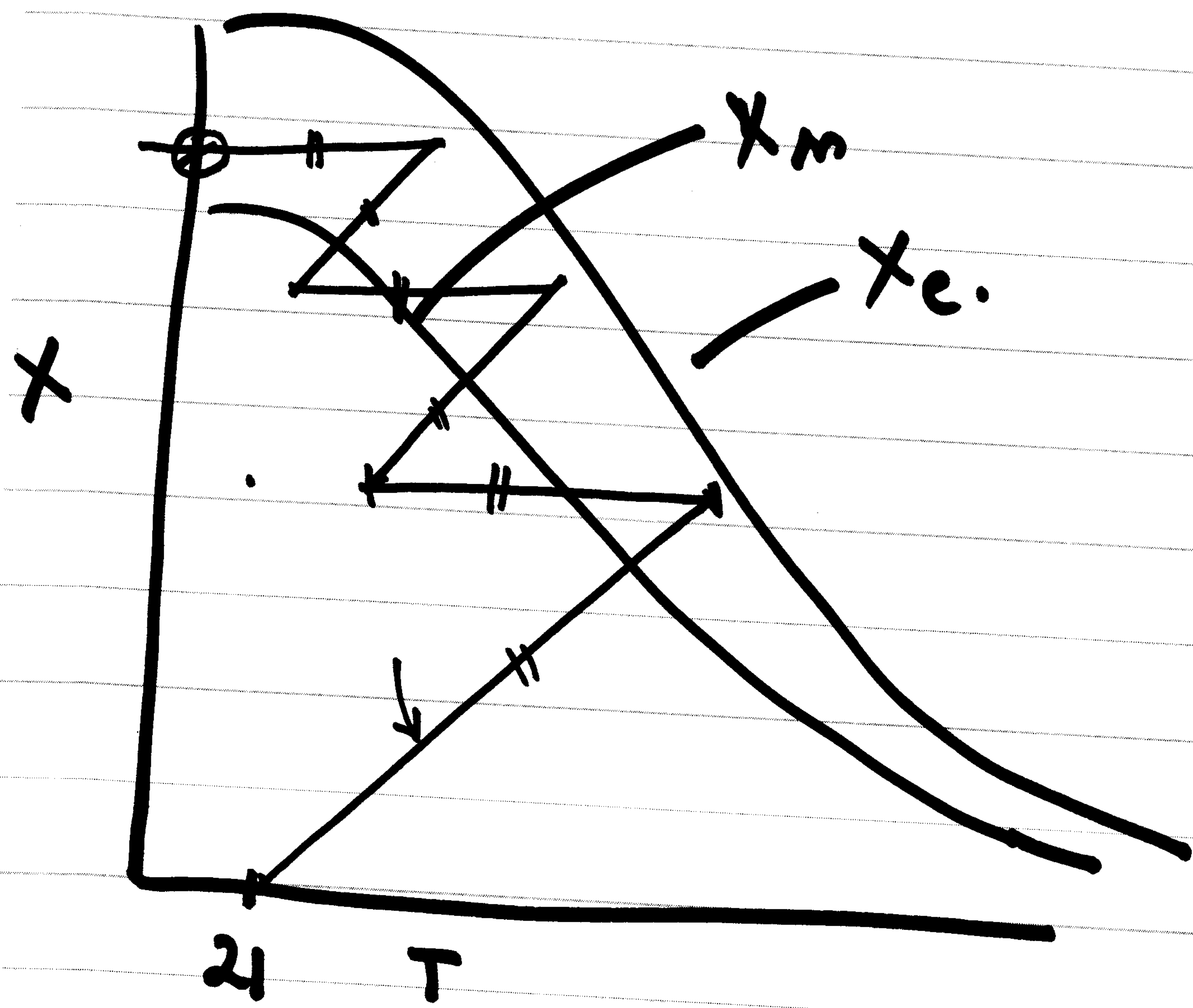
$\Delta H = -20,000 \frac{cal}{mol}$

$k = 12/hr$ @ 21C

$K = 12.2$ @ 25C



$$E_1 - E_2 = \Delta H_r$$

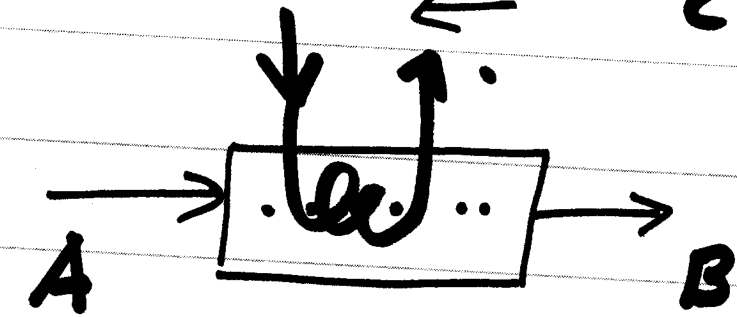


$$X_e = \frac{K}{K+1}$$

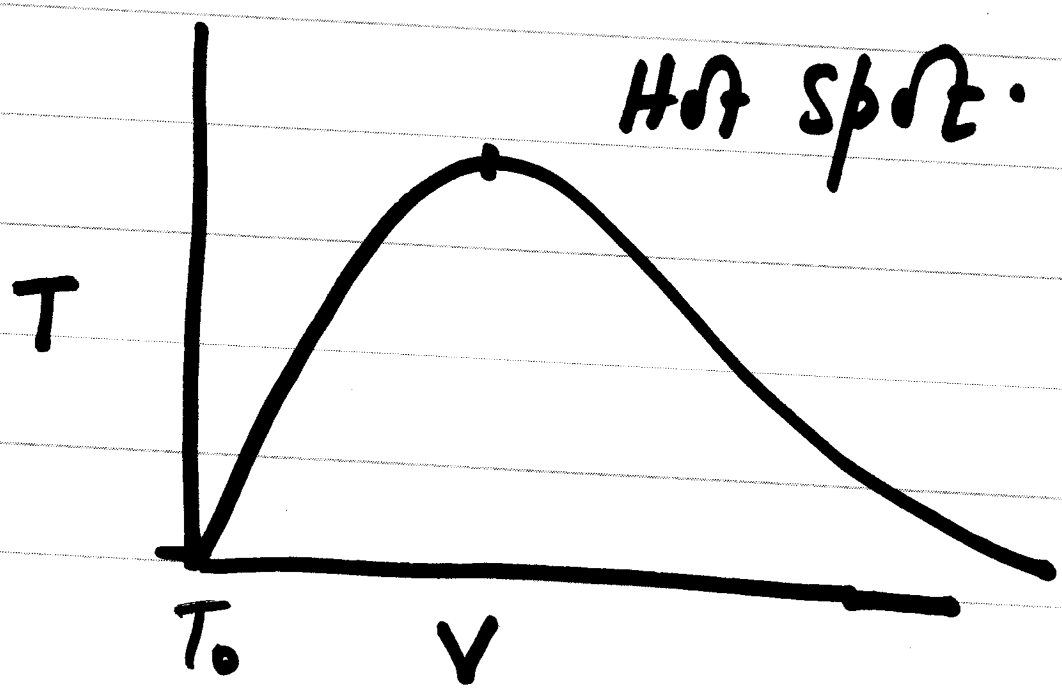
$$\frac{X_m}{1-X_m} = \frac{KE_1}{E_2}$$

$$\frac{dT}{dx} = \frac{C_{A0}(-\Delta H_1^{*})}{C_p}$$

$A \rightleftharpoons B$ Exo



Hot spot.



Max permissible hot spot.

Mole

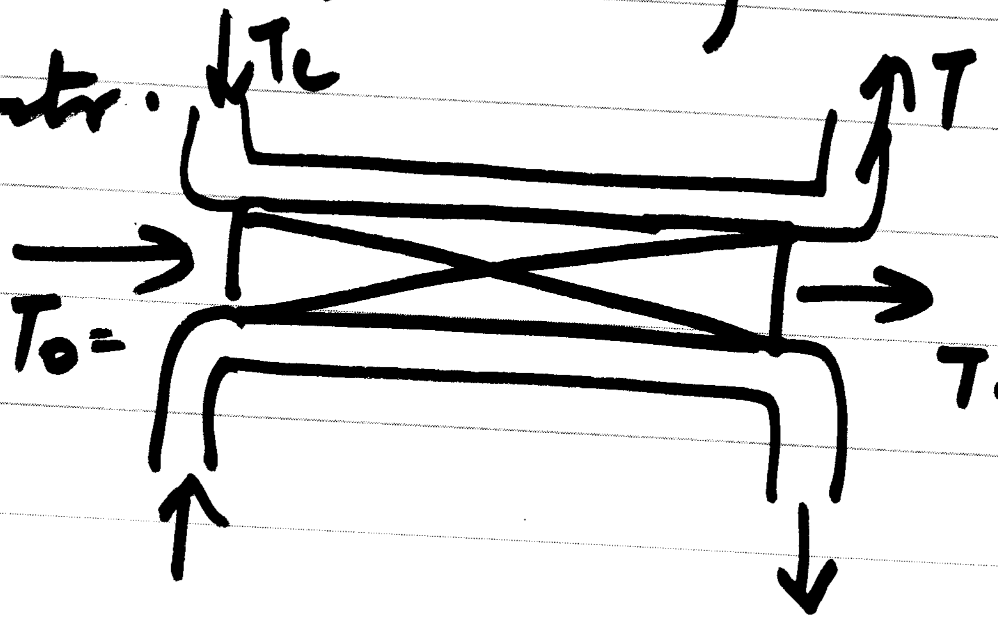
$$F_{A0} \frac{dx}{dV} = r_1 - r_2$$

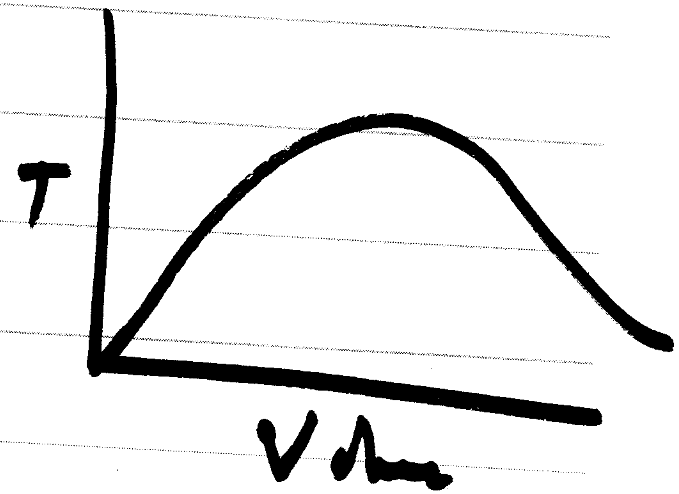
$$v C_p \frac{dT}{dV} = (r_1 - r_2)(-\Delta H_1^*) + \cdots - W_s$$

$$+ q - W_s$$

$$q = \frac{4h}{D}(T_c - T).$$

Constant temperature operation of a Tubular catalytic Reactor.





$$A \rightarrow B$$

Mole Balance

$$\frac{dF_A}{dV} = r_B$$

$$= k_1 \alpha C_{A0} (1-x)$$ α: Cat activity

$$\frac{dx}{d\tau} = k_1 \alpha C_{A0} (1-x)$$

Energy Balance

$$v C_p \frac{dT}{dx} = k_1 \alpha C_{A0} (1-x) (-\Delta H_1^*) + q.$$

$$\frac{dx}{d\tau} = k_1 \alpha C_A (1-x).$$

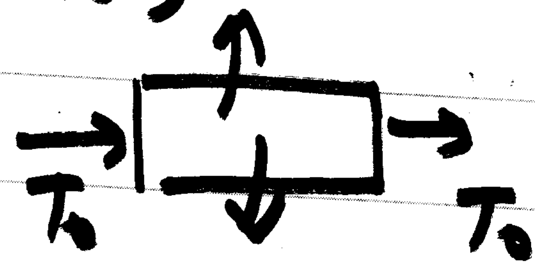
$$v C_p \cancel{\frac{dT}{dV}} = k_1 \alpha C_{A0} (1-x)(-\Delta H^*) + q \underset{q}{\cancel{- W_s}}$$

$$0 = k_1 \alpha C_{A0} (1-x)(-\Delta H^*) + \frac{4h}{D}(T_c - T).$$

$$0 = k_1(T,V)\, \alpha(T,V)\, C_{A0} \left[1 - x(T,V)\right](-\Delta H^*) + \frac{4h}{D}(T_c - T)$$

$$q = \frac{4h}{D}\left(T_c - T\right).$$

$$-q = k_1 \alpha\, C_{A0}(1-x)(-\Delta H^*) \quad \text{—(2)}$$



We also know

$$(-q)\,V = \overbrace{F_{A0}(-\Delta H^*)}\,x$$

$$x = \frac{-qV}{F_{A0}(-\Delta H^*)} = \frac{-q\,\tau}{C_{A0}(-\Delta H^*)} \quad \text{—(4)}$$

$$-q = k_1 \alpha C_{A0} \left[1 + \frac{q \tau}{C_{A0}(-\Delta H_1^*)} \right]$$

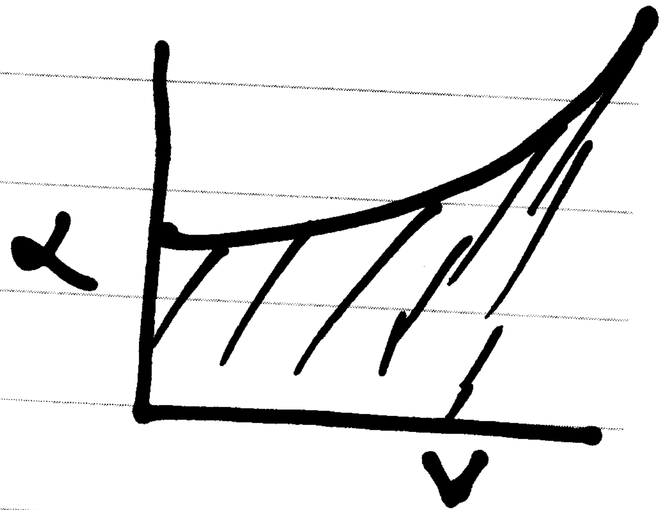
$$\alpha = \frac{(-q/k_1)}{C_{A0}\left[1 + \frac{q \tau}{C_{A0}(-\Delta H_1^*)} \right]}$$

$$(\alpha) = \frac{\left[-q/h\right](-\Delta h^*)}{(-\Delta h^*)\,c_m + q\tau}$$

$T = 290$

$C_{A0} = \checkmark \qquad v_0 = \checkmark$

$$\alpha = \frac{(-q/k_1)(-\Delta H_1^*)\, v_0}{v_0(-\Delta H^*)C_{A0} + qV}$$



$$\alpha = \frac{v_0\,(-q/k_1)\,(-\Delta H_1^*)}{v_0(-\Delta H^*)\,C_{A0} + qV}$$