Prof. Shankar

Lec. 38 9/12/2012

10 Dec

~~15 Dec~~ 16 Dec

Advanced Reaction Engineering

Practice Problems in Gas Solid Reactions

Sponge Iron Technology

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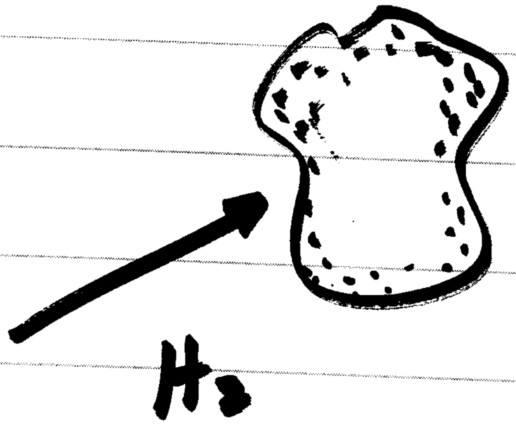
Sponge Iron

$$Fe_2O_3 + 3H_2 = 2Fe + 3H_2O$$

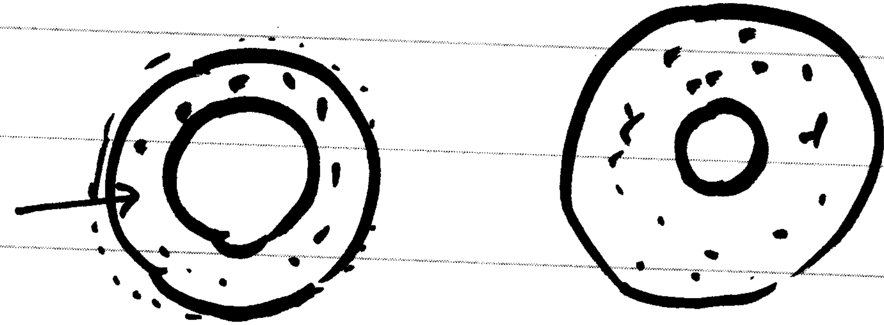
b B(S) (A)

K_p at 25C = 0.1

Heat of Rxn = (+) 7 kcal/mol.

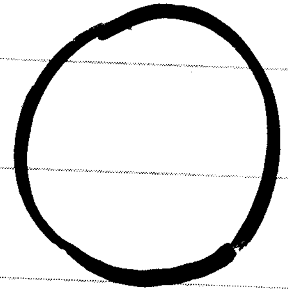


Shrinking Core



Ext Diffusion
Int. Diffusion (Product layer)
Rxn.

$A(g) + bB(s) \rightarrow \text{Products}$



$$t = \tau_R \left(1 - \frac{r_c}{R}\right) + \tau_F \left(1 - r_c^3/R^3\right) + \tau_D \left[1 - 3\left(\frac{r_c}{R}\right)^2 + 2\left(r_c/R\right)^3\right]$$

$$\left(\frac{r_c}{R}\right) = \left(1 - X_B\right)^{1/3}$$

$$t = \tau_R \left(1 - \frac{r_c}{R}\right) + \tau_F \left(1 - r_c^3/R^3\right) + \tau_D \left\{1 - 3 r_c^2/R^2 + 2 r_c^3/R^3\right\}$$

$$\tau_R = \rho_B R / b k_s C_{Ag}$$

$$\tau_F = \rho_B R / 3 b k_g C_{Ag}$$

$$\tau_D = \rho_B R^2 / 6 b D C_{Ag}$$

ρ_B = particle density

R : particle size

C_{Ag} : Conc gas in contact with solid

k_s - Reaction

k_g - mass TC

D : Diffusion coeff

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$k_s = (1.93)\,10^5 \exp(-12000/T)$ cm/s

D_e : product layer (for hydrogen) = 0.03 cm^2/s

k_g = Film diffusion Coeff : 10 cm/s

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K_p at 600 C

$$\ln \frac{K_{p_2}}{K_{p298}} = -\frac{\Delta H}{R}\left[\frac{1}{T} - \frac{1}{298}\right]$$

$\Delta H = (+)\ 7$ Kcal/mol.

K_p (600 c) = 228.

$$Fe_2O_3 + 3H_2 = 2Fe + 3H_2O\ (g)$$
(s)

$$K_p = p^3_{H_2O}/(p_{H_2})^3$$

7 $\frac{A(g)}{3} + \frac{B(s)}{3} = \frac{2C(s)}{3} + \frac{3D(g)}{3}$

~~Kp~~ =

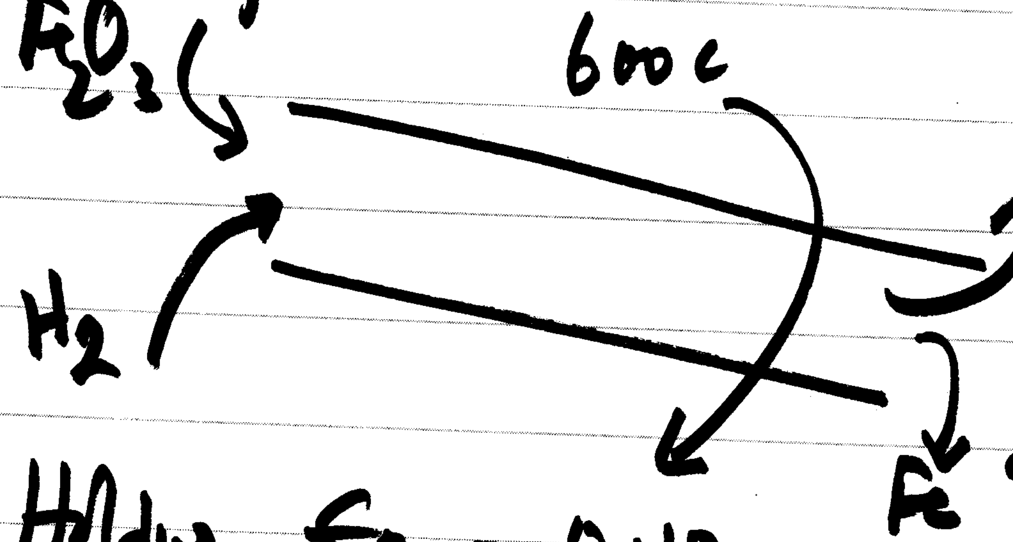
$F_A = F_{A0}(1 - X_A)$

$F_D = $ ~~F_{D0}~~ $+ F_{A0} X_A$

$$K_p = \left[\frac{(C_{A0} X_A^*) RT}{C_{A0}(1 - X_A^*) RT} \right]^3 = \frac{X_A^{*3}}{(1 - X_A^*)^3} = K_p = 228$$

Solve $X_A^* = 0.86 \Rightarrow$ equilibrium Conversion

2mm particles



$X_A^* = 0.86$

$X_A = (0.95)\,X_A^*$

Holdup $\epsilon_R = 0.10$

95% eq. conversion

$$\ln\left[X_A^* - X_A\right] = \frac{3\,k_g\,\epsilon_R\,\tau_g}{R}$$

Putting numbers. $\tau_g = 0.2\,s.$

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Solid Residence time

$$\frac{V}{v_s} = \left(\tau_g \frac{v_g}{v_s}\right)$$

$$= \tau_g \left(\frac{F_{A0}}{C_{A0}}\right)\left(\frac{C_{B0}}{F_{B0}}\right)$$

$F_{A0} = F_{B0}$ (given)

Putting numbers $\tau_s = \underline{\underline{285s}}$

习题 10

$$Fe_2O_3 + 3H_2 = 2Fe + 3H_2O$$

$$\frac{F_{A0} X_A}{F_{B0}} = 3 X_B$$

$$X_A = 0.95\, X_A^*$$

$$X_B = \frac{2}{3} X_A = \frac{2}{3}(0.95)(0.88) \qquad X_A^* = 0.88$$

$$X_B = 0.55.$$

$$1 - X_B = \frac{r_c^3}{R^3} \Rightarrow \left(\frac{r_c}{R}\right) = 0.766.$$

''

$$t = 10700(1 - 0.761)$$

$$+ 71(1 - 0.45)$$

$$+ 5952\{1 - 3(0.761)^2 + 2(0.761)^3]$$

$$= 3333 \text{ Seconds} \simeq 1 \text{ hour}$$

$$C_{Ag} = \frac{P}{RT} = \frac{1\,atm}{(0.082)(873)} = (0.014)\,10^{-3}\ mol/m^3$$

$$t = \tau_R\left(1-\frac{r_c}{R}\right) + \tau_F\left(1-\frac{r_c}{R^3}\right) + \tau_D\left(1-3\frac{r_c^2}{R^2}+2\frac{r_c^3}{R^3}\right)$$

$R = 5\,mm$

$X_A = 0.95\,X_A^*$

$$\tau_R = \frac{\rho_B R}{b k_s C_{Ag}} = \text{Putting numbers} = 10700\ s.$$

$(r_c/R = 0.766)$

$$\tau_F = \frac{\rho_B R}{3 b k_g C_{Ag}} = \text{Putting numbers} = 71\ s.$$

$$\tau_D = \frac{\rho_B R^2}{6 b D C_{Ag}} = 5952\ s.$$

Advanced Reaction Engineering.

Practice Problem in RTD.

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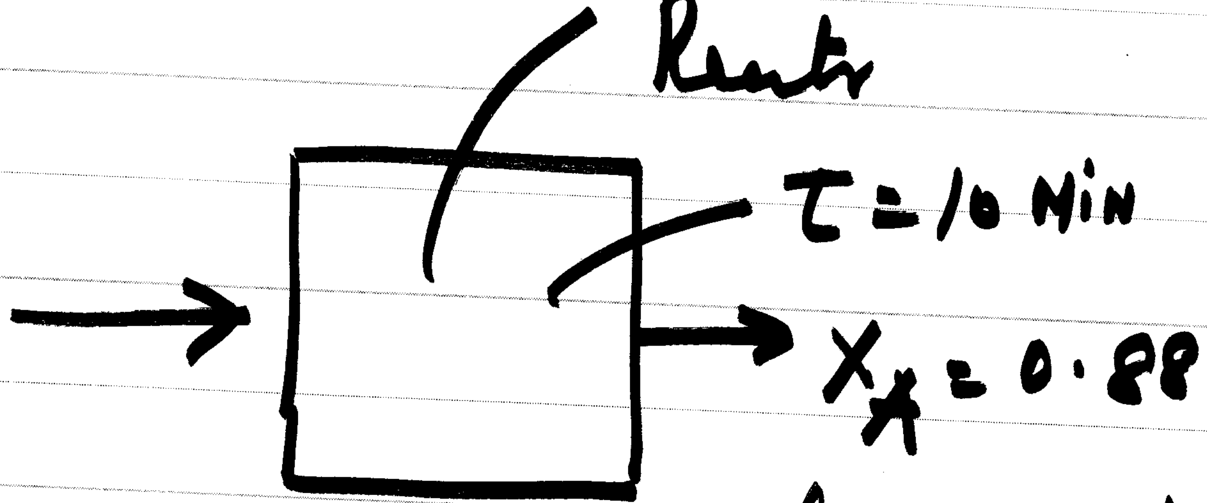
$A \rightarrow B$



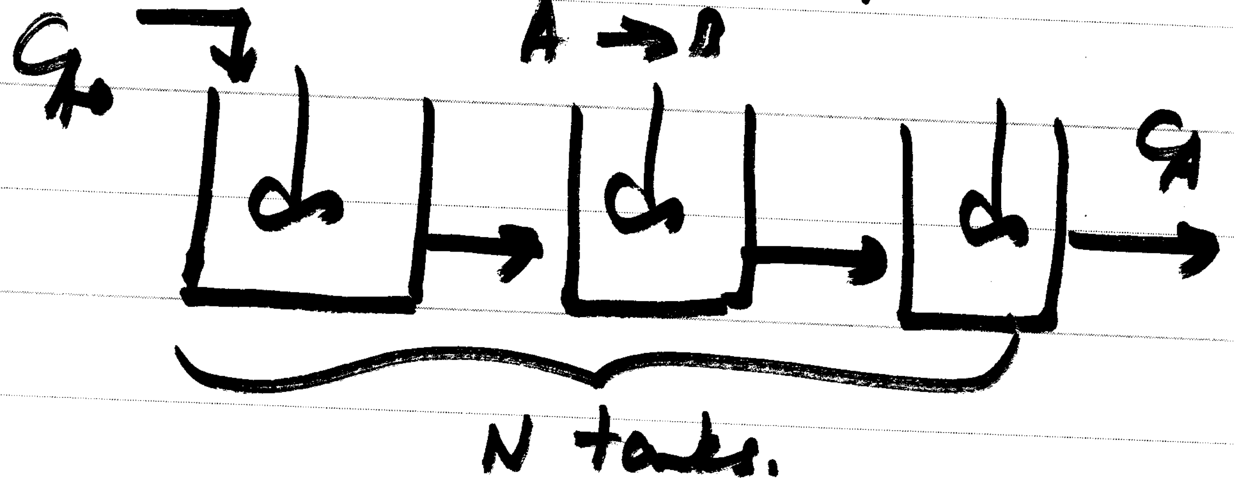
$k = 0.3/\text{Min.}$

(1) Tanks in Series. [N]

(2) Dispersion Model

(3) Recycle Reactor Model

Tanks in Series Model



$X_A = 0.8$

$\tau = 10\ \text{MIN}$

$k = 0.3/\text{MIN}$

$$\left(\frac{C_A}{C_{A0}}\right) = \frac{1}{\left(1 + \frac{k\tau}{N}\right)^N}$$

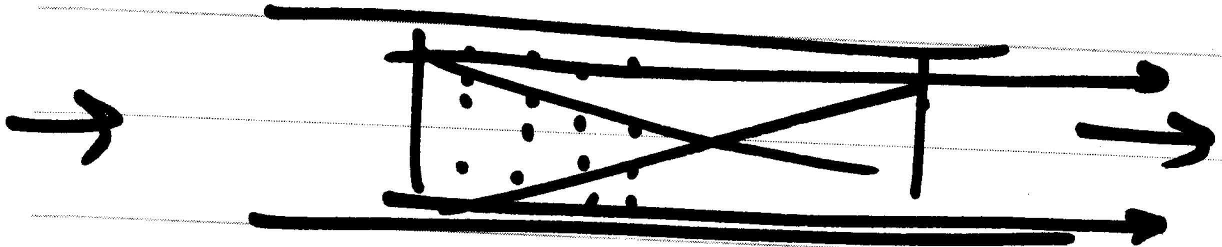
$$1 - 0.88 = \frac{1}{\left(1 + \frac{(0.3)(10)}{N}\right)^N}$$

Solve for N

$= 3.3$

Dispersion Model. → $X_A = 0.88$

$A \rightarrow B$ $\quad k = 0.3/\text{min}$



$\tau = 10$ min.

$$\frac{C_A}{C_{A0}} = \frac{4q\, e^{Pe/2}}{(1+q)^2 \exp\left(\frac{Pe\, q}{2}\right) - (1-q)^2 \exp\left(-\frac{Pe\, q}{2}\right)}.$$

$q : 1 + 4\frac{Da}{Pe}$ $\qquad Da : k\tau$

$1 - 0.88 =$

Putting numbers find Pe

LHS = 0.12

$Pe \simeq 10$ roughly <u>LHS = RHS</u>.

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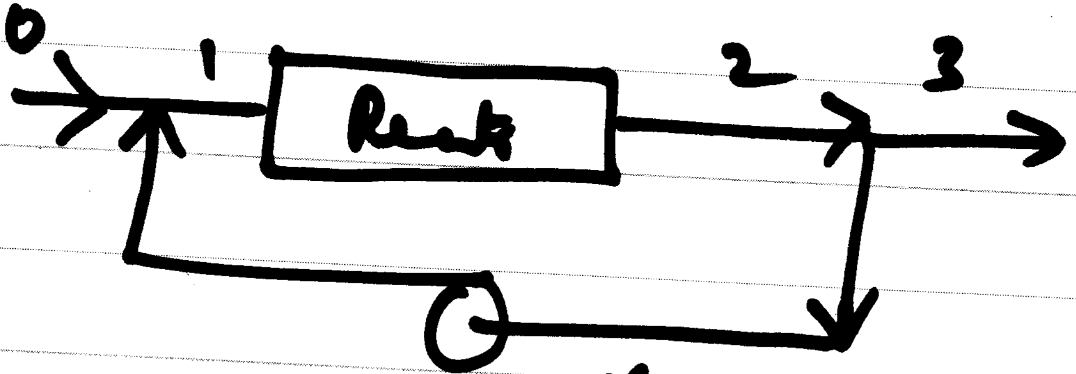
Recycle Reactor



$R = 0$ PFR

$R = \infty$ CSTR

$$\frac{V}{F_{A0}} = (R+1)\int_{\frac{R}{R+1}X_3}^{X_3} \frac{dx}{-r_A}$$

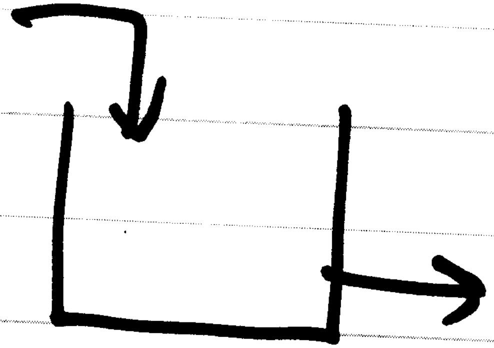
A 18

$$\frac{k\tau}{(R+1)} = \ln\left[\frac{1 + R\, C_A/C_{A0}}{(C_A/C_{A0})(R+1)}\right]$$

$C_A/C_{A0} = 0.88$; $k = 0.3/\text{min}$

$\tau =$ ~~10/min~~ 10 Min.

Plotting makes Sure $R = 0.9$.



$X_A = 0.8f$

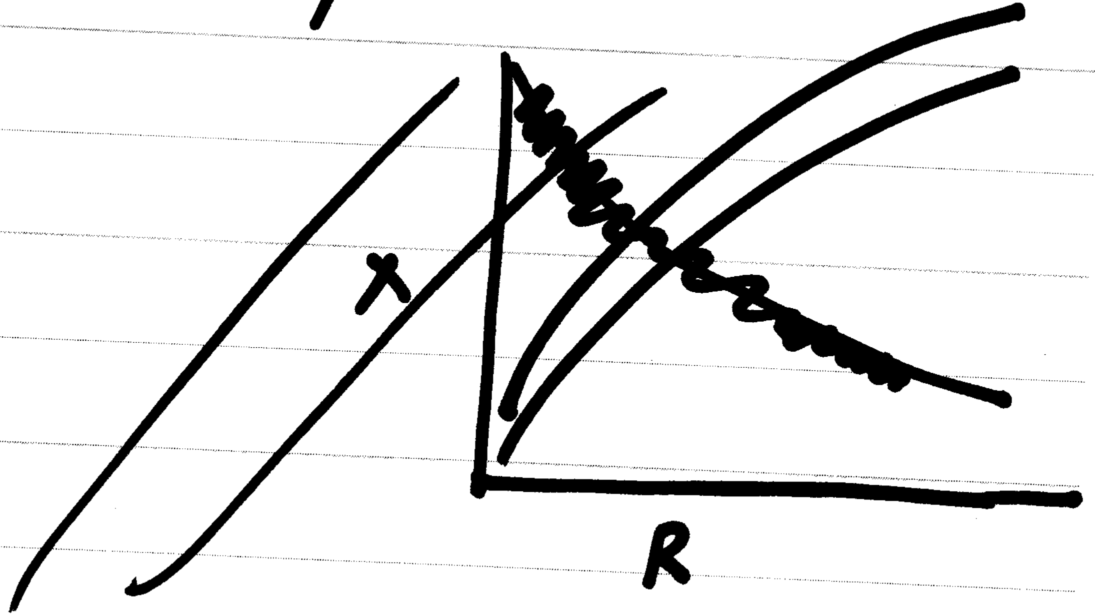
$\tau = 10$ MIN

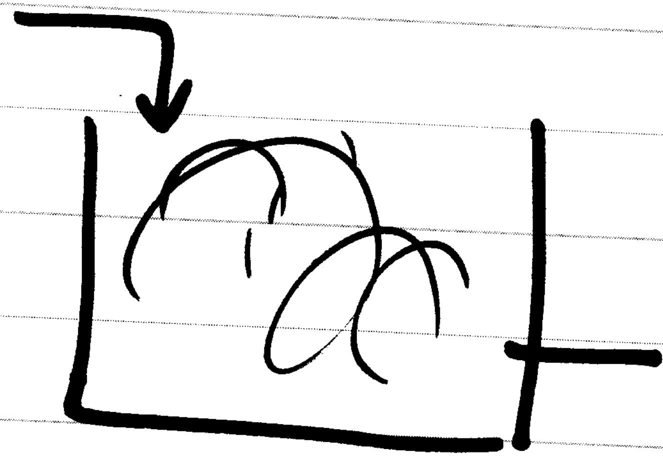
$k = 0.3/\text{min}$

$Pe = 10$

$N = 3.3$

$R = 0.9$





$x_A = 0.88$

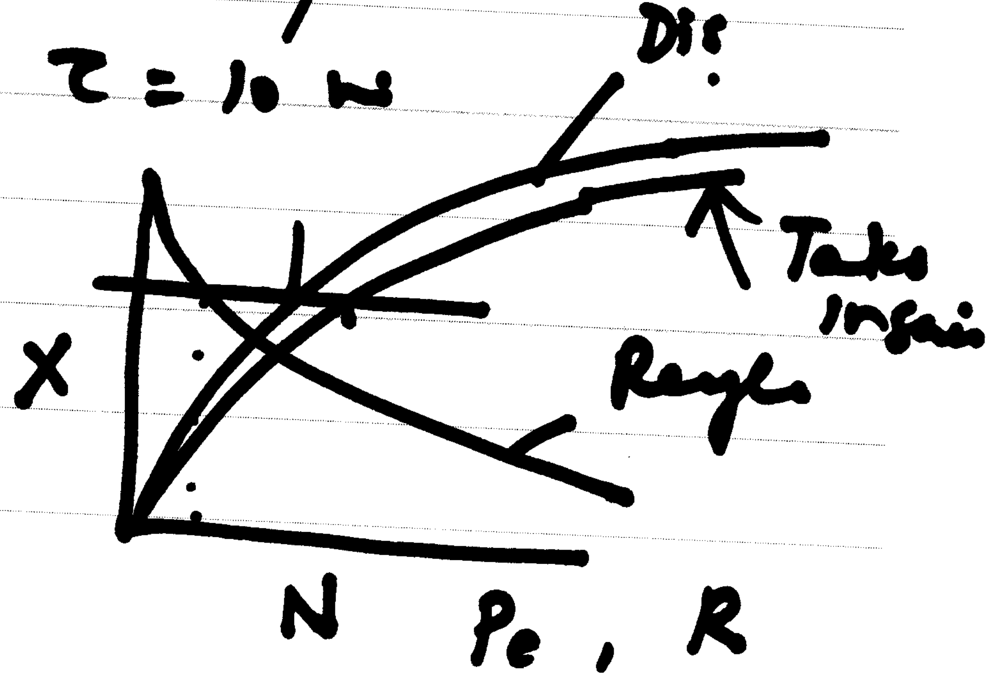
$k = 0.3/\text{min}$

$\tau = 10 \text{ min}$

$N = 3.3$

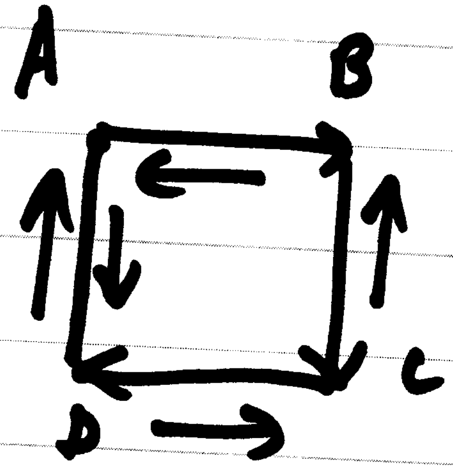
$Pe \simeq 10$

$R = 0.9$



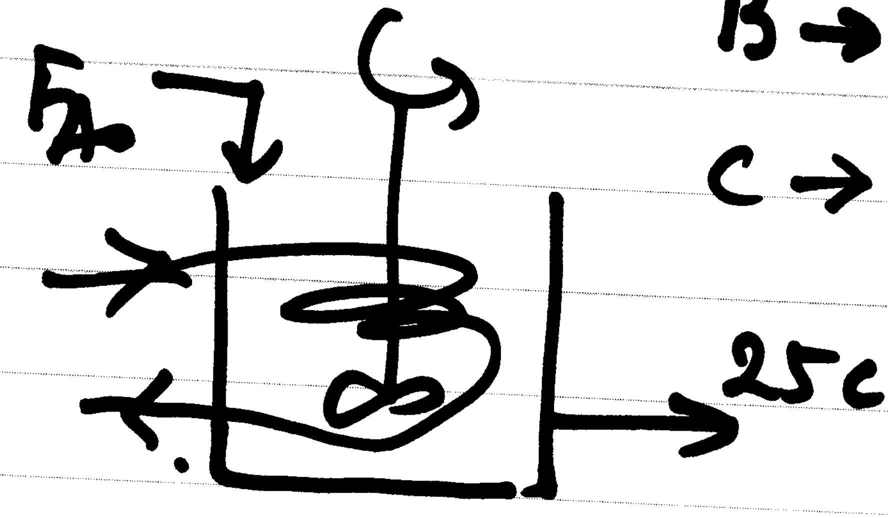
Advanced Reaction Engineering

Reaction Network Analysis.



Kcal/mol

A → B	$K_1 = 1$	$\Delta H_1 = 10$
B → C	$K_2 = 2$	$\Delta H_2 = 20$
C → D	$K_3 = 3$	$\Delta H_3 = 30$



1) All Reaction are intantaneous

2) T = 25.C

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$A \rightarrow B \quad X_1$

$B \rightarrow C \quad X_2$

$C \rightarrow D \quad X_3$

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

$F_B = F_{A0}(X_1 - X_2)$

$F_C = F_{A0}(X_2 - X_3)$

$F_D = F_{A0} X_3$

$\frac{C_B}{C_A} = K_1$

$\frac{C_C}{C_B} = K_2$

$\frac{C_D}{C_C} = K_3$

$$C_B = \frac{F_B}{v} = \frac{F_{A0}(X_1 - X_2)}{v_0}$$

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

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

$$C_C = \frac{F_C}{v} = \frac{F_{A0}(X_2 - X_3)}{v_0} = C_{A0}(X_2 - X_3)$$

$$C_D = \frac{F_D}{v} = \frac{F_{A0}(X_3)}{v_0} = C_{A0} X_3.$$

$$\frac{C_B}{C_A} = 1.0 = K_1$$

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

$$X_1 - X_2 = 1 - X_1 \Rightarrow$$

$$2X_1 = 1 - X_2 \qquad X_1 = \frac{1 - X_2}{2}$$

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$$\frac{c_2}{c_1} = K_2 = 2$$

$$\frac{x_2 - x_3}{x_1 - x_2} = 2.$$

$$\frac{c_3}{c_2} = K_3 = 3$$

$$\frac{x_3}{x_2 - x_3} = 3$$

$$x_3 = 3x_2 - 3x_3$$

$$4x_3 = 3x_2$$

$$x_3 = 0.75x_2$$

$$\frac{x_2 - x_3}{x_1 - x_2} = 2$$

Solving

$x_1 = 0.9$

$x_2 = 0.8$

$x_3 = 0.6.$