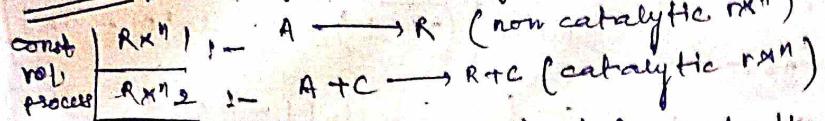


12/02/24

Homogenous catalytic rxns: (post midsem)



Let C_A be the conc of reactant A, C_c be the conc of catalyst (applicable to rxn 2)

$$(r_A)_{\text{net}} = (-r_A)_{\text{non-catalytic}} + (-r_A)_{\text{catalytic rxn}}$$

$$= k_1 C_A + k_2 C_A C_c$$

$$= C_A (k_1 + k_2 C_c)$$

$$\frac{-1}{V} \frac{dV}{dt} = C_A (k_1 + k_2 C_c)$$

$$\frac{dC_A}{dt} = C_A (k_1 + k_2 C_c) \quad \begin{cases} k_1, k_2 \text{ are the} \\ \text{rxn rate constants} \\ C_c = \text{fixed} \end{cases}$$

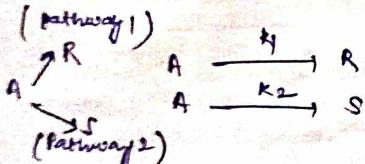
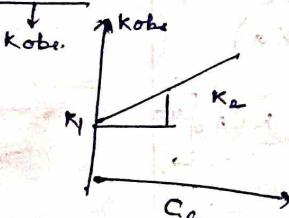
$$\Rightarrow - \int_{C_{A0}}^{C_A} \frac{dC_A}{C_A} = -(k_1 + k_2 C_c) \int_0^t dt$$

$$\Rightarrow \left\{ \ln \left(\frac{C_A}{C_{A0}} \right) \right\}_{C_{A0}}^{C_A} = (k_1 + k_2 C_c) t$$

$$\Rightarrow -\ln \left| \frac{C_{A0}(1-x_A)}{C_A} \right| = (k_1 + k_2 C_c) t$$

$$\Rightarrow -\ln (1-x_A) = (k_1 + k_2 C_c) t$$

$$\begin{cases} k_{\text{obs}} = k_1 + k_2 C_c \\ y = c + mx \end{cases}$$



$$-r_A = -\frac{1}{V} \frac{dV}{dt} = k_1 C_A + k_2 C_A$$

$$\Rightarrow -\frac{dC_A}{dt} = (k_1 + k_2) C_A$$

$$\Rightarrow \int_{C_{A0}}^{C_A} -\ln C_A = (k_1 + k_2) t$$

$$\Rightarrow -\ln \left| \frac{C_A}{C_{A0}} \right| = (k_1 + k_2) t$$

~~So, a straight line plot of $\ln \left(\frac{C_A}{C_{A0}} \right)$ vs time~~

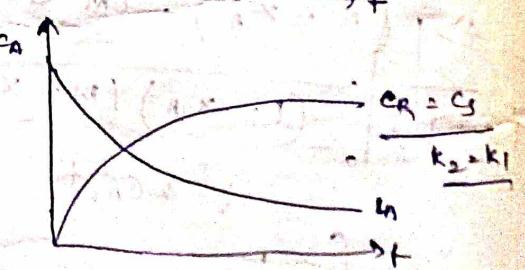
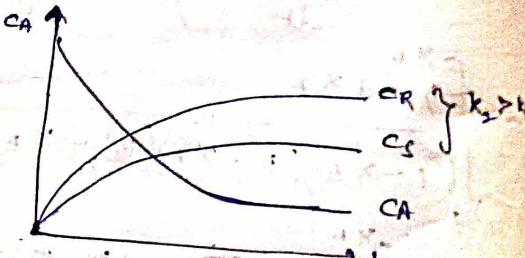
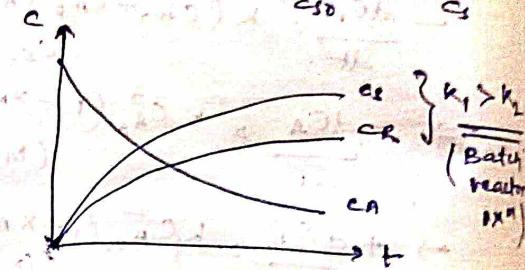
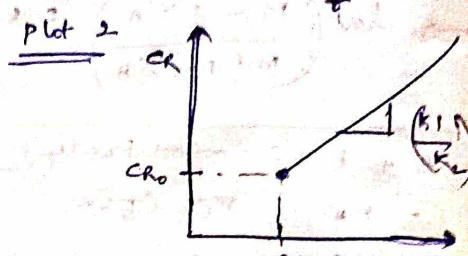
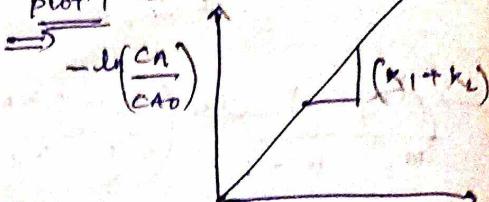
$$r_R = \frac{dC_R}{dt} = k_1 C_A$$

$$r_S = \frac{dC_S}{dt} = k_2 C_A$$

$$\frac{r_R}{r_S} = \frac{dC_R/dt}{dC_S/dt} = \frac{k_1}{k_2}$$

$$\text{OR} \int dC_R = \frac{k_1 f(C_S)}{k_2} dC_S$$

$$\Rightarrow \left(\frac{C_R - C_{R0}}{C_S - C_{S0}} \right) = \frac{k_1}{k_2}$$



$$-r_A = k C_A^a C_B^b$$

How to det. half-life of a rxn?

$$C_B = f(C_A)$$

$$\alpha, \beta \rightarrow \frac{C_B}{C_A} = \frac{\beta}{\alpha} \rightarrow C_B = \left(\frac{\beta}{\alpha} \right)^{C_A}$$

$$\Rightarrow (-r_A) = k C_A^a \left(\frac{\beta}{\alpha} \right)^b C_A^b$$

$$\Rightarrow (-r_A) = k \left(\frac{\beta}{\alpha} \right)^b C_A^{a+b}$$

$\frac{d}{dt}$ = a th order w.r.t A
 $\frac{d}{dt}$ = b th order w.r.t B
 $n = (a+b)$ = overall order of the rxn.
 $- \frac{dC_A}{dt} = k C_A^n$
 $\int - \frac{dC_A}{dt} dt = \int k C_A^n dt \Rightarrow \left[\frac{-C_A}{(-n+1)} \right]_{C_{A_0}}^{C_A} = kt$
 $\Rightarrow \left[\frac{1}{(n-1) C_A^{1-n}} \right]_{C_{A_0}}^{C_A} = \frac{k}{n-1} t$
 $= \frac{1}{(n-1)} \left\{ \frac{\circlearrowleft}{C_A^{1-n}} - \frac{\circlearrowleft}{C_{A_0}^{1-n}} \right\} = \frac{k}{n-1} t$
 $\Rightarrow \frac{1}{(n-1)} \left\{ \frac{\circlearrowleft}{C_A^{1-(a+b)}} - \frac{\circlearrowleft}{C_{A_0}^{1-(a+b)}} \right\} = \frac{k}{n-1} t$
 $\Rightarrow \frac{\circlearrowleft}{C_A^{1-(a+b)}} - \frac{\circlearrowleft}{C_{A_0}^{1-(a+b)}} = \frac{k}{n-1} t [a+b-1]$
 $\text{at } t = t_{1/2}$
 $\Rightarrow \left\{ \frac{C_{A_0}}{C_A} \right\}^{\frac{1-a-b}{1-a-b}} = \frac{C_{A_0}}{C_A}$
 $\Rightarrow \left(\frac{C_{A_0}}{C_A} \right)^{\frac{1-a-b}{1-a-b}} = \frac{k}{n-1} t_{1/2}$
 $\Rightarrow \left(\frac{C_{A_0}}{C_A} \right)^{\frac{1-a-b}{1-a-b}} = \frac{k}{n-1} t_{1/2}$
 $\Rightarrow t_{1/2} = C_{A_0} \left[\frac{1-a-b}{k(n-1)} \right]$
 $\rightarrow \log t_{1/2} = (1-\eta) \log C_{A_0} + \log \left\{ \frac{1-\eta}{k(n-1)} \right\}$
 $y = mx + c$
 $\log t_{1/2} = (1-\eta) \log C_{A_0} + \log \left\{ \frac{0.5}{k(n-1)} \right\}$
 $y = \log t_{1/2}, x = \log C_{A_0}$

26/02/24

Shifting orders n^{th} :

$A \rightarrow R$ [Non elementary rxn.]
 rate expression: $-r_A = k_1 C_A$

conditions:

- C_A is high: $k_2 C_A \gg 1$
- C_A is low: $r_A = \frac{k_1 C_A}{k_2 C_A}$

$\Rightarrow r_A = \frac{k_1 C_A}{k_2 C_A} = k_1 C_A$ (zeroth order rxn.)

C_A is low. $\Rightarrow 1 > k_2 C_A$

$\Rightarrow r_A = k_1 C_A = k_1 C_A$

first order rxn: $\frac{1}{V} \frac{dN_A}{dt} = \frac{k_1 C_A}{1+k_2 C_A}$

$\Rightarrow -\frac{dC_A}{dt} = \frac{k_1 C_A}{1+k_2 C_A}$

$\Rightarrow \frac{(1+k_2 C_A)}{k_1 C_A} dC_A = -\frac{1}{V} dt$

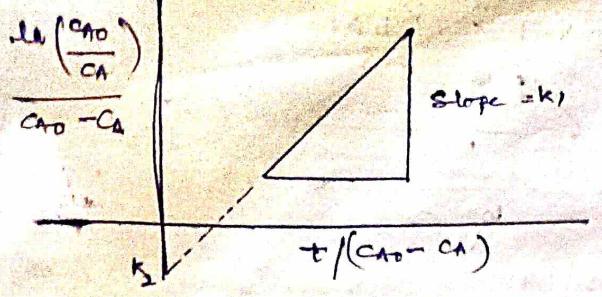
$\Rightarrow \sqrt{\frac{1}{k_1 C_A} dC_A + \frac{k_2}{k_1} dC_A} = -\frac{1}{V} t$

$\Rightarrow \left[\frac{1}{k_1} dC_A + \frac{k_2}{k_1} dC_A \right] = -\frac{1}{V} t$

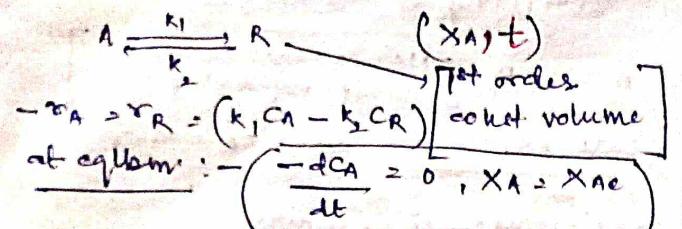
$\Rightarrow \frac{1}{k_1} \ln \left| \frac{C_A}{C_{A_0}} \right| + \frac{k_2}{k_1} (C_A - C_{A_0}) = -\frac{1}{V} t$

$\Rightarrow \ln \left| \frac{C_{A_0}}{C_A} \right| = \frac{k_1 + k_2}{C_{A_0} - C_A} - \frac{k_2}{k_1}$

$\Rightarrow \frac{\ln \left| \frac{C_{A_0}}{C_A} \right|}{(C_{A_0} - C_A)} = -\frac{k_2}{k_1} + \frac{k_1 + k_2}{C_{A_0} - C_A}$



reversible rxns



$$\Rightarrow -r_A = k_1 (C_{AO} - C_A X_A) - k_2 \left[\frac{C_{AO} C_A}{C_{AO}} \right]$$

$$\Rightarrow \frac{C_{AO}}{C_{AO}} = M$$

$$\Rightarrow -r_A = k_1 C_{AO} (1 - X_A) - k_2 [M C_{AO} + C_{AO} X_A]$$

$$\Rightarrow \frac{-dC_A}{V dt} = k_1 C_{AO} (1 - X_A) - k_2 [M C_{AO} + C_{AO} X_A]$$

$$\Rightarrow \frac{dC_A}{dt} = k_1 C_{AO} (1 - X_A) - k_2 [M C_{AO} + C_{AO} X_A]$$

$$\frac{dx_A}{dt} = \frac{k_1}{(M + X_{Ae})} (M + 1) (X_{Ae} - X_A) \quad \text{find like terms}$$

$$\Rightarrow \frac{d(C_{AO} - C_A)}{dt} =$$

$$\Rightarrow \frac{dC_A}{dt} = k_1 C_{AO} (1 - X_A) - k_2 [M + X_A] C_{AO}$$

$$\Rightarrow \frac{-dX_A}{dt} = k_1 (1 - X_A) - k_2 (M + X_A)$$

$$\text{and after rearranging } \Rightarrow k_2 = \left(\frac{1 - X_{Ae}}{M + X_{Ae}} \right) k_1$$

$$\Rightarrow \frac{-dX_A}{dt} = k_1 (1 - X_A) - k_2 (M + X_A)$$

$$\Rightarrow \frac{-dX_A}{dt} = dt$$

$$\Rightarrow \frac{-k_2 (M + X_A) + k_1 (1 - X_A)}{dt}$$

$$\begin{aligned} & \frac{-dX_A}{(k_1 - k_2 M) - X_A (k_1 + k_2 M)} = dt \\ & \Rightarrow \frac{-dX_A}{(k_1 + k_2) X_A} = \frac{(k_1 + k_2)}{k_1 - k_2 M} dt \\ & \Rightarrow \ln \left(1 - \frac{(k_1 + k_2) X_A}{k_1 - k_2 M} \right) = -(k_1 + k_2) t \\ & \Rightarrow 1 - \left(\frac{(k_1 + k_2)}{k_1 - k_2 M} \right) X_A = e^{-(k_1 + k_2) t} \\ & \Rightarrow X_A = \left[\frac{1 - e^{-(k_1 + k_2) t}}{\left(\frac{k_1 - k_2 M}{k_1 + k_2} \right)} \right] \end{aligned}$$

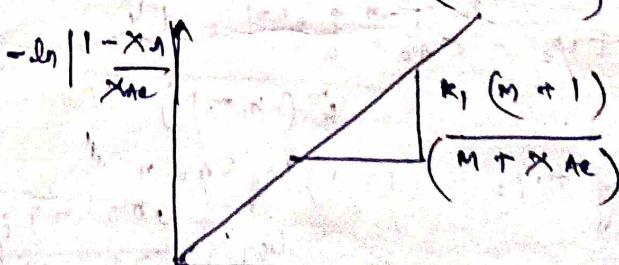
$$\frac{dX_A}{(X_{Ae} - X_A)} = \frac{k_1 (M + 1)}{M + X_{Ae}} dt$$

$$\Rightarrow \left[-\ln |X_{Ae} - X_A| \right]_0^X_A = \frac{k_1 (M + 1)}{M + X_{Ae}} t$$

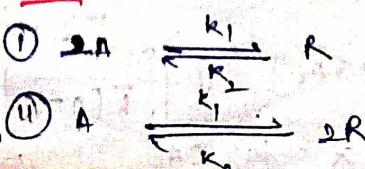
$$\Rightarrow -\ln |X_{Ae} - X_A| + \ln |X_{Ae}| = \frac{k_1 (M + 1)}{M + X_{Ae}} t$$

$$\Rightarrow -\ln \left| \frac{X_{Ae} - X_A}{X_{Ae}} \right| = \frac{k_1 (M + 1)}{(M + X_{Ae})} t$$

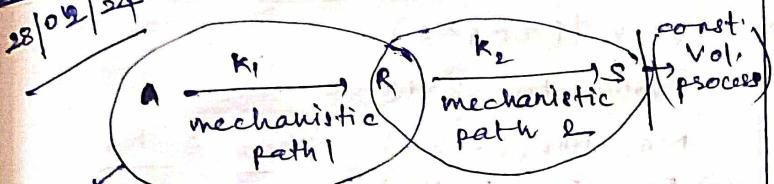
$$\Rightarrow -\ln \left| \frac{1 - X_A}{X_{Ae}} \right| = \frac{k_1 (M + 1)}{(M + X_{Ae})} t$$



MW



28/02/24



$c_A(t)$, $c_R(t)$, $c_S(t) \rightarrow$ to optimum $\rightarrow c_{R,\text{mix}}$

$$\begin{aligned} -n_A &= k_1 c_A \quad (I) \\ -n_R &= k_1 c_A - k_2 c_R \quad (II) \\ n_S &= k_2 c_R \quad (III) \end{aligned}$$

$$\frac{-dc_A}{dt} = k_1 c_A$$

$$\int_{c_A(0)}^{c_A(t)} \frac{dc_A}{c_A} = k_1 \int_0^t dt$$

$$\Rightarrow (-\ln c_A)_{c_A(0)} = k_1 t$$

$$\Rightarrow \ln \left(\frac{c_A}{c_{A0}} \right) = -k_1 t \rightarrow c_A = c_{A0} e^{-k_1 t}$$

$$n_R = k_1 c_A - k_2 c_R$$

$$\frac{dc_R}{dt} + k_2 c_R = k_1 c_A = k_1 c_{A0} e^{-k_1 t}$$

$$\int_{c_R(0)}^{c_R(t)} \frac{dc_R}{dt} + k_2 c_R = k_1 c_{A0} e^{-k_1 t} dt$$

$$\Rightarrow e^{\int_{c_R(0)}^{c_R(t)} \frac{dc_R}{dt} + k_2 c_R} = k_1 c_{A0} e^{-k_1 t} \int_{c_R(0)}^{c_R(t)} k_2 dt$$

$$\Rightarrow \frac{d}{dt} [c_R e^{k_2 t}] = k_1 c_{A0} e^{(k_2 - k_1)t}$$

$$\Rightarrow \int d [c_R e^{k_2 t}] = \int k_1 c_{A0} e^{(k_2 - k_1)t} dt$$

$$\Rightarrow c_R e^{k_2 t} = \frac{k_1 c_{A0} e^{(k_2 - k_1)t}}{(k_2 - k_1)} + c \rightarrow \text{const.}$$

$$\Rightarrow c = c_{R0} - \frac{k_1 c_{A0}}{(k_2 - k_1)}$$

$$\Rightarrow c = -\frac{k_1 c_{A0}}{k_2 - k_1}$$

$$c_R e^{k_2 t} = \frac{k_1 c_{A0} e^{(k_2 - k_1)t}}{(k_2 - k_1)} - \frac{k_1 c_{A0}}{(k_2 - k_1)}$$

$$\Rightarrow c_R e^{k_2 t} = \frac{k_1 c_{A0}}{k_2 - k_1} \left[e^{(k_2 - k_1)t} - 1 \right]$$

$$\Rightarrow c_R = \frac{k_1 c_{A0}}{k_2 - k_1} e^{-k_2 t} \left[\frac{e^{k_2 t} - 1}{e^{k_2 t}} \right]$$

$$\Rightarrow c_R = \frac{k_1 c_{A0}}{(k_2 - k_1)} \left[\frac{e^{k_2 t} - e^{k_1 t}}{e^{k_1 t}} \right] e^{k_1 t}$$

$$\Rightarrow c_R = \frac{k_1 c_{A0}}{k_2 - k_1} \left[1 - \frac{e^{-k_2 t} \cdot e^{k_1 t}}{e^{k_1 t}} \right]$$

$$\Rightarrow c_R = \frac{k_1 c_{A0}}{(k_2 - k_1)} \left[e^{-k_1 t} - e^{-k_2 t} \right]$$

$$\Rightarrow c_R = \frac{k_1 c_{A0}}{(k_2 - k_1)} \left[\frac{e^{-k_1 t} - e^{-k_2 t}}{k_2 - k_1} \right]$$

$$\text{Now, } c_{A0} = c_A + c_R + c_S$$

$$\Rightarrow c_{A0} - c_A - c_R = c_S$$

$$\Rightarrow c_{A0} - c_{A0} e^{-k_1 t} - k_1 c_{A0} \left[\frac{e^{-k_1 t} - e^{-k_2 t}}{(k_2 - k_1)} \right] = c_S$$

$$\frac{d}{dt}(c_R) = 0$$

$$\Rightarrow \frac{dC_R}{dt} = k_1 C_{A0} e^{-k_1 t} + k_1 C_{A0} (k_2 - k_1) e^{-k_2 t}$$

$$\Rightarrow \frac{dC_R}{dt} = \frac{k_1^2 C_{A0} e^{-k_1 t}}{k_2 - k_1} - \frac{k_1 k_2 C_{A0} e^{-k_2 t}}{k_1 - k_2}$$

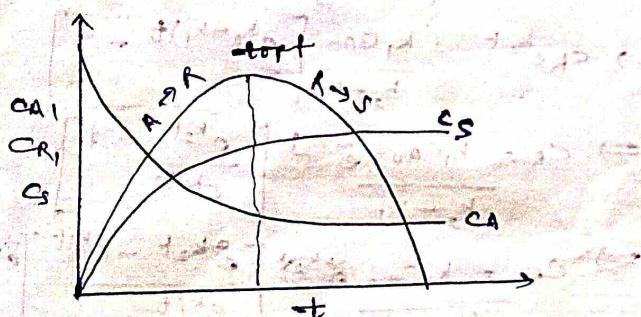
$$\Rightarrow 0 = \frac{-k_1^2 C_{A0} e^{-k_1 t}}{k_2 - k_1} + \frac{k_1 k_2 C_{A0} e^{-k_2 t}}{k_1 - k_2}$$

$$\Rightarrow \frac{k_1^2 C_{A0} e^{-k_1 t_{opt}}}{k_2 - k_1} = \frac{k_1 k_2 C_{A0} e^{-k_2 t_{opt}}}{k_1 - k_2}$$

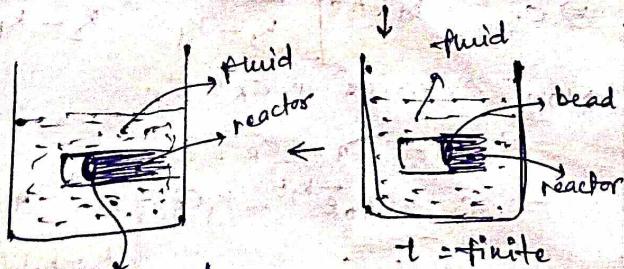
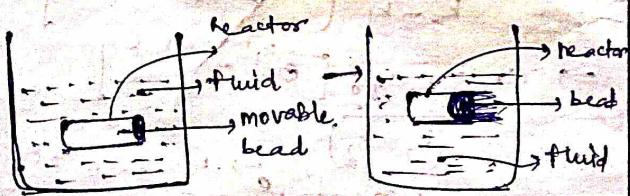
$$\Rightarrow t_{opt} = \ln \left(\frac{k_2}{k_1} \right)$$

$$\frac{dC_R}{dt} + k_2 C_{R,\max} = k_1 C_{A0} e^{-k_1 t_{\max}}$$

$$\Rightarrow C_{R,\max} = \frac{C_{A0}}{\left(\frac{k_1}{k_2} \right) \left(\frac{k_2 - k_1}{k_1} \right)}$$



29/02/24
Variable Volume Batch Reactor



Volume $V = V_0(1 + \epsilon_A x_A) \rightarrow$ Clear relationship between ϵ_A & x_A

$V = \text{Vol. of the reactor } (t = t_0)$

$V_0 = \text{Initial vol. of the reactor } (t = 0) \Rightarrow \frac{dV}{dt}$

$\epsilon_A = \text{Vol. Expansion factor}$

$x_A = \text{fractional conversion}$

$$\epsilon_A = \frac{V/x_A - 1}{V/x_A} = 0$$

$$= \frac{\text{Vol. of the reactor at } x_A=0 - \text{Vol. of the reactor at } x_A=1}{\text{Vol. of the reactor at } x_A=0}$$



$$\epsilon_A = ?? = \frac{4-1}{1} = 3.$$

50% A
50% I

$$1A \rightarrow 4R + 1I$$

$$= \frac{5-2}{2} = \frac{3}{2} = 1.5$$

$$V = V_0 (1 + \epsilon_A x_A)$$

volumetric feed rate

$$N_A = N_{A0} (1 - x_A) \quad \frac{C_{A0}}{V_0} = \frac{F_A}{V_0}$$

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

$C_A = C_{A0} (1 - x_A)$
molw/time

$$\frac{N_A}{V} = \frac{C_A}{V}$$

$$\Rightarrow \frac{N_{A0} (1 - x_A)}{V_0 (1 + \epsilon_A x_A)} = \frac{C_A}{V}$$

variable vol. process

$$C_A = \frac{C_{A0} (1 - x_A)}{(1 + \epsilon_A x_A)}$$

$$\text{const. } \frac{dC_A}{dx_A} \rightarrow C_A = C_{A0} (1 - x_A) \rightarrow dC_A = \frac{C_{A0}}{dx_A}$$

dC_A for vari. vol. :-

$$\frac{dC_A}{dx_A} \text{ process}$$

$$-\frac{dC_A}{dx_A} = \frac{F_A \epsilon_A C_{A0}}{V_0} \left[(1 + \epsilon_A x_A)^{-1} - \frac{(1 - x_A) \epsilon_A}{(1 + \epsilon_A x_A)^2} \right]$$

$$\Rightarrow \frac{dC_A}{dx_A} = C_{AO} \left[\frac{e_A x_A - e_A - 1 - e_A x_A}{(1 + e_A x_A)^2} \right] \Rightarrow \frac{-C_{AO}(1 + e_A)}{(1 + e_A x_A)^2}$$

v & t (zero-order)

$$-\frac{1}{V} \frac{dN_A}{dt} = -r_A = k \Rightarrow -\frac{1}{V_0(1 + e_A x_A)} \frac{d}{dt} [N_{AO}(1 - x_A)] = k$$

$$\Rightarrow \frac{N_{AO}}{V_0(1 + e_A x_A)} \frac{dx_A}{dt} = k \Rightarrow \frac{C_{AO}}{1 + e_A x_A} \frac{dx_A}{dt} = k \Rightarrow \frac{dx_A}{1 + e_A x_A} = \frac{k dt}{C_{AO}}$$

$$\Rightarrow \frac{1}{e_A} \int_0^{x_A} \frac{e_A dx_A}{1 + \frac{x_A e_A}{C_{AO}}} = \frac{k}{C_{AO}} \int_0^t dt \Rightarrow \ln |1 + e_A x_A| = \frac{k t}{C_{AO}}$$

$$\Rightarrow \ln |1 + e_A x_A| = \frac{k t + C_1}{C_{AO}} \quad \left\{ \begin{array}{l} v = V_0(1 + e_A x_A) \\ \frac{v}{V_0} = 1 + e_A x_A \end{array} \right\}$$

$$\Rightarrow \ln \left| \frac{v}{V_0} \right| = \frac{k e_A t}{C_{AO}}$$

(first order)

$$-\frac{1}{V} \frac{dN_A}{dt} = -r_A = k C_A \Rightarrow -\frac{1}{V_0(1 + e_A x_A)} \frac{d}{dt} [N_{AO}(1 - x_A)] = -\frac{k N_A}{V} N_A$$

$$\Rightarrow \frac{N_{AO}}{V_0(1 + e_A x_A)} \frac{dx_A}{dt} = \frac{k N_A (1 - x_A)}{V_0(1 + e_A x_A)} \Rightarrow \int_0^{x_A} \frac{dx_A}{1 - x_A} = \int_0^t k dt$$

$$\Rightarrow \ln |1 - x_A| = kt$$

$$\Rightarrow \ln \left| 1 - \frac{\Delta V}{V_0 e_A} \right| = kt \quad \left\{ \begin{array}{l} N_A = N_{AO}(1 - x_A) \\ \frac{v}{V_0} = 1 + e_A x_A \Rightarrow \frac{v - 1}{V_0} = e_A x_A \end{array} \right.$$

$$\Rightarrow x_A = \frac{\Delta V}{V_0 e_A}$$

(second order)

$$-\frac{1}{V} \frac{dN_A}{dt} = k C_A^2 \Rightarrow -\frac{1}{V_0(1 + e_A x_A)} \frac{d}{dt} [N_{AO}(1 - x_A)] = k \left(\frac{N_A}{V} \right)^2$$

$$\Rightarrow \frac{N_{AO}}{V_0(1 + e_A x_A)} \frac{dx_A}{dt} = \frac{k N_{AO} (1 - x_A)^2}{V_0^2 (1 + e_A x_A)^2} \Rightarrow \frac{dx_A}{(1 - x_A)^2} = \frac{k N_A dt}{V_0 (1 + e_A x_A)}$$

$$\Rightarrow \int_0^{x_A} \frac{1 + e_A x_A}{(1 - x_A)^2} dx_A = k C_{AO} \int_0^t dt \Rightarrow \int_0^{x_A} \frac{1 + e_A x_A}{(1 - x_A)^2} dx_A = k C_{AO} t$$

$$\Rightarrow \frac{(1 + e_A) \Delta V}{V_0 e_A - \Delta V} + e_A \ln \left(\frac{1 - \frac{\Delta V}{V_0 e_A}}{1 + e_A x_A} \right) = k C_{AO} t$$

$$C_A = \frac{P_A}{V_0} = \frac{P_{AO}(1-x_A)}{V_0} = C_{AO}(1-x_A)$$

$$C_B = \frac{P_B}{V_0} = \frac{P_{AO}\left(B_B - \frac{b}{a}x_A\right)}{V_0} = C_{AO}\left(B_B - \frac{b}{a}x_A\right)$$

$$C_C = \frac{P_C}{V_0} = \frac{P_{AO}\left(B_C + \frac{c}{a}x_A\right)}{V_0} = C_{AO}\left(B_C + \frac{c}{a}x_A\right)$$

$$C_D = \frac{P_D}{V_0} = \frac{P_{AO}\left(B_D + \frac{d}{a}x_A\right)}{V_0} = C_{AO}\left(B_D + \frac{d}{a}x_A\right)$$

$$CI = \frac{F_I}{V_0} = \frac{P_{AO} \cdot T}{V_0} = C_{AO} \cdot P_I$$

Variable Vol. process :-

$$\log PV = N_R R T \quad \text{compressibility factor} \quad \text{--- (1)}$$

$$P_0 V_0 = N_R R T_0 \cdot Z_0$$

$$\frac{PV}{P_0 V_0} = \frac{N_R R T}{N_R R T_0} \left(\frac{Z}{Z_0}\right)$$

$$\rightarrow V = \frac{P_0 V_0}{P} \frac{N_R}{N_R} \left(\frac{Z}{Z_0}\right) T \left(\frac{\frac{Z}{Z_0}}{T_0}\right)$$

$$\rightarrow V = V_0 \frac{N_R P_0 T}{N_R P T_0} \left(\frac{\frac{Z}{Z_0}}{T_0}\right)$$

$$\rightarrow V = V_0 \left(\frac{1 + \epsilon A_0 x_A}{N_R} \right) \frac{P}{P_0} \frac{T}{T_0} \frac{\frac{Z}{Z_0}}{T_0}$$

$$\text{Now } \delta Y_{AO} = \epsilon, \quad \frac{N_T - N_{T_0}}{N_T}$$

$$\text{when } x_A = 1, \quad [\delta = \left(\frac{d}{a} + \frac{c}{a} \right) - \left(1 + \frac{b}{a} \right)]$$

$$\epsilon \text{ reduces to } \frac{N_T - N_{T_0}}{N_T}$$

$$[\text{at } x_A = 1, \quad N_T = N_{T_f}]$$

$$\Rightarrow \epsilon = N_{T_f} - N_{T_0}$$

$$= \text{change in total no. of moles at } x_A = 1$$

Initially (no. of moles fed to the system)

$$\Rightarrow V = V_0 \left(\frac{Z}{Z_0} \right) \left(\frac{T}{T_0} \right) \left(\frac{P_0}{P} \right) (1 + \epsilon x_A)$$

for gas phase x_A 's, T and P are such that $Z \approx Z_0$

$$\Rightarrow V = V_0 \left(\frac{T}{T_0} \right) \left(\frac{P_0}{P} \right) (1 + \epsilon x_A)$$

further simplification gives :-

$$V = V_0 (1 + \epsilon x_A)$$

Now, find out the expressions for C_A , C_B , C_C , C_D , CI :-

$$C_A = \frac{N_A}{V} = \frac{N_A (1 - x_A)}{V_0 (1 + \epsilon x_A) \left(\frac{T}{T_0} \right) \left(\frac{P_0}{P} \right)}$$

$$\Rightarrow C_A = \frac{C_{AO} (1 - x_A)}{(1 + \epsilon x_A) \left(\frac{T_0}{T} \right) \left(\frac{P_0}{P} \right)}$$

$$C_B = \frac{C_{AO} \left(1 - \frac{b}{a} x_A \right)}{(1 + \epsilon x_A) \left(\frac{T_0}{T} \right) \left(\frac{P_0}{P} \right)}$$

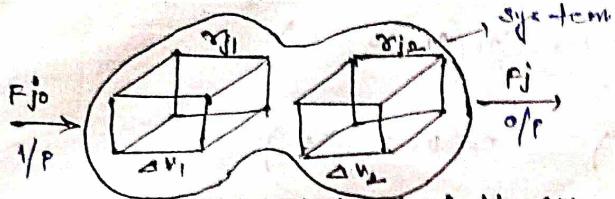
$$C_C = \frac{C_{AO} \left(1 + \frac{c}{a} x_A \right)}{(1 + \epsilon x_A) \left(\frac{T_0}{T} \right) \left(\frac{P_0}{P} \right)}$$

$$C_D = \frac{C_{AO} \left(1 + \frac{d}{a} x_A \right)}{(1 + \epsilon x_A) \left(\frac{T_0}{T} \right) \left(\frac{P_0}{P} \right)}$$

HW → find floweqs. eq's

F_A	F_B	F_C	F_D	F_I
C_A	C_B	C_C	C_D	CI

General mole balance eqn :-



$$\frac{I}{P} = \frac{O}{P} + \text{disappearance} \\ \text{chemical rxn} \\ + \text{accumulation}$$

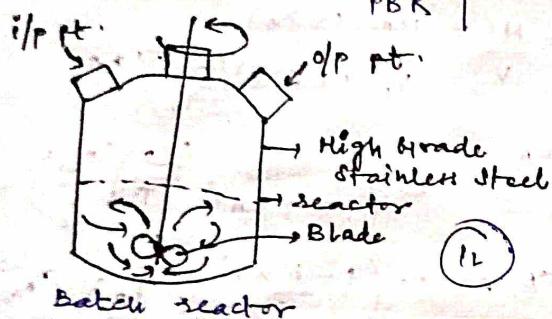
rate of molar flow in moles/time

+ rate of gen' = rate of
of pdt. molar flow (mole)
out (moles/time)

$$\Rightarrow Fj_0 + \int r_j dV = Fj + \frac{dN_j}{dt}$$

In batch sps., there is no Fj_0 & Fj .

unsteady state \rightarrow Batch reactor
steady state \rightarrow PFR CSTR PBR



small scale production

expensive pdt.

Advantage:- High conversion can be achieved if we allow the rxn to continue for longer period of time.

Disadvantages:- (i) High investment
(ii) Variability of the pdt. from batch to batch.

(iii) Time consuming process

rate of gen' = rate of accumul'

$$(ii) V = \frac{dN_A}{dt} = \frac{dN_{A_0}}{dt} (1 - X_A)$$

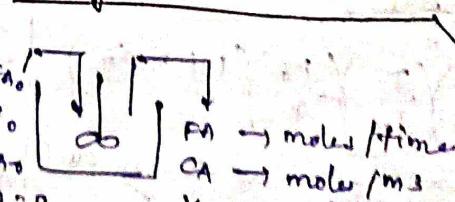
$$(ii) V = N_{A_0} \frac{dX_A}{dt}$$

$$\rightarrow (-r_A)V = N_{A_0} \frac{dX_A}{dt}$$

$$\Rightarrow \int_0^{X_A} N_{A_0} dX_A = - \int_0^t dt$$

$$\Rightarrow N_{A_0} \int_0^{X_A} \frac{dX_A}{(-r_A)V} = t$$

Performance eqn of
a batch reactor



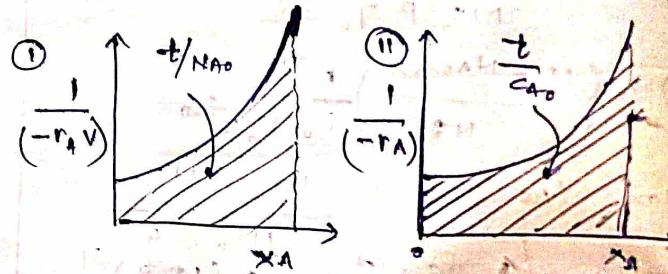
rate of inflow = rate of outflow + rate of generation
= rate of accumulation
 \Rightarrow Inflow - outflow + rate of gen' = 0

when there is no spatial variation
(uniform mixing)

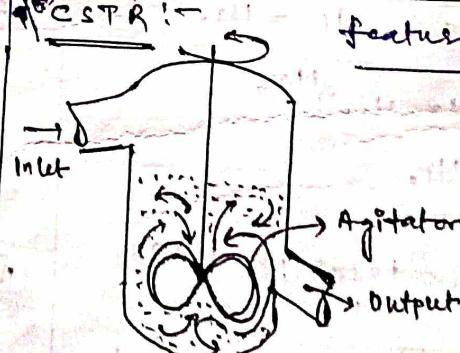
$$\text{Now, } t = \frac{N_{A_0}}{V} \int_0^{X_A} \frac{dX_A}{(-r_A)}$$

$$t = \frac{C_{A_0}}{V} \int_0^{X_A} \frac{dX_A}{(-r_A)} \quad \rightarrow \text{for const. vol. process}$$

$$t = \frac{N_{A_0}}{V} \int_0^{X_A} \frac{dX_A}{(-r_A)(1 + t_{eq} X_A)} \quad \rightarrow \text{variable vol. proc.}$$



CSTR !



features:- (i) operated in steady state.

(ii) mostly liquid phase reactions performed in CSTR

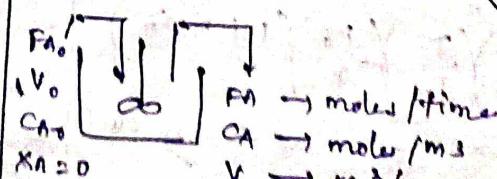
(iii) Perfect Mixing

(iv) No spatial variation in conc, Temp, etc.

(v) Conc inside conc at any pt. inside CSTR

at any pt. inside CSTR
the s = at the reactor outlet

Mixing Pattern in a CSTR



rate of inflow = rate of outflow + rate of generation

= rate of accumulation

\Rightarrow Inflow - outflow + rate of gen' = 0

$$\Rightarrow F_{j0} - F_j + (r_j)v = \frac{dN}{dt} \xrightarrow{>0}$$

$$\Rightarrow F_{j0} - F_j = -(r_j)v$$

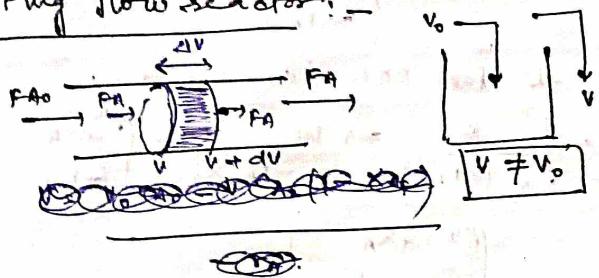
$$\Rightarrow v = \frac{|F_{j0} - F_j|}{(-r_j)}$$

$$\Rightarrow v = \frac{F_{A0} - F_A}{-r_A} = \frac{v_0 C_{A0} - v C_A}{(-r_A)}$$

$$\Rightarrow F_{A0} = v_0 C_{A0}, F_A = v C_A$$

$$v = \frac{v_0 C_{A0} - v C_{A0}(1 - x_{Af})}{(-r_A)}$$

Plug flow reactor:-



$$F_{A0} - F_A + (r_A)v = \frac{dN_A}{dt}$$

ΔV element is very small & there is no change in reaction rate at any pt. inside the ΔV element. Then, we can write:-

$$\Rightarrow F_A |_{V} - F_A |_{V+\Delta V} + (r_A) \Delta V \approx 0$$

$$\Rightarrow - [F_A |_{V+\Delta V} - F_A |_V] + r_A \Delta V \approx 0$$

$$\Rightarrow \frac{F_A |_{V+\Delta V} - F_A |_V}{\Delta V} \approx r_A$$

$$\Rightarrow \frac{dF_A}{dV} = r_A \Rightarrow \int dF_A = \int \frac{dV}{r_A}$$

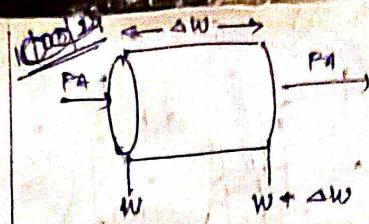
$$\Rightarrow F_{A0} \int_{0}^{X_A} \frac{dX_A}{(-r_A)} = V$$

$$\Rightarrow \frac{V}{F_{A0}} = \int_{0}^{X_A} \frac{dX_A}{-r_A} \Rightarrow \frac{V}{V_0 C_{A0}} = \int_{0}^{X_A} \frac{dX_A}{(-r_A)}$$

$$\Rightarrow \frac{T}{C_{A0}} = \int_{0}^{X_A} \frac{dX_A}{(-r_A)}$$

$$T = \text{residence time} = \frac{V}{V_0} = \frac{\text{time}}{\text{space vel.}}$$

$$\text{Space vel.} = \frac{1}{T} = \text{time}^{-1}$$



$$\Rightarrow \frac{w}{w + \Delta w} = \frac{1}{W} \frac{dW}{dt}$$

moles of A
(mass of catalyst)
(time)
Homogeneous
rate

11/08/24 Performance Eq's :-

$$\text{Batch reactor: } \frac{t}{N_{A0}} = \int_0^t \frac{dX_A}{(-r_A)v}$$

$$\text{CSTR: } \frac{V}{F_{A0}} = \frac{X_A}{(-r_A)v_{exit}}$$

$$\text{PFR: } \frac{V}{F_{A0}} = \frac{T}{C_{A0}} = \int_0^T \frac{dX_A}{(-r_A)}$$

initial
P_A
 $X_A = 0$
LHSV packed
bed
min

$$\text{PBR: } \frac{W}{F_{A0}} = \int_0^{X_A} \frac{dX_A}{(-r_A)}$$

wt. of catalyst
per unit time product

at the entrance conditions.

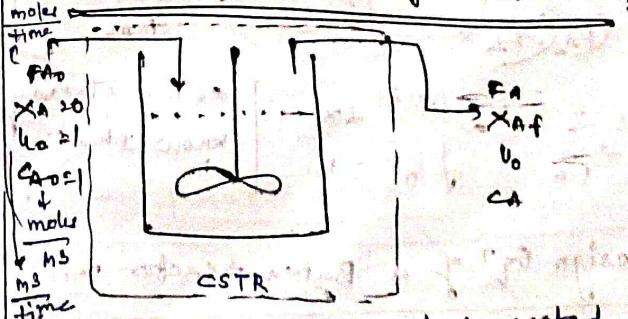
$$\text{Space Vel.} = \frac{V_0}{V}$$

Liq. hourly space Vel. = Bas hourly space
Vel. (LHSV)

$$\frac{V_0}{V} \text{ at } 60^\circ\text{F}$$

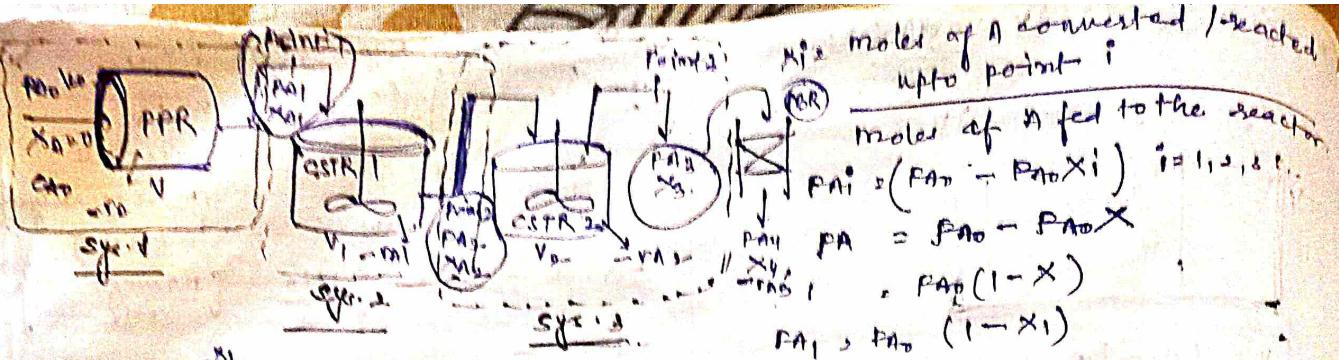
V = 2 m³
T = 2 m³ / 0.01 m³/s : s
STP

Conversion for a single reactor

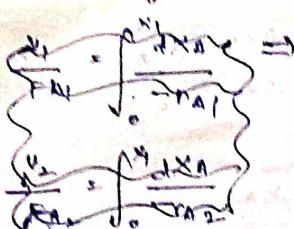


$$\text{conversion} = \frac{\text{moles of A reacted}}{\text{moles of A fed to the reactor}}$$

$$\approx \left(1 - \frac{CA_f}{CA_0}\right) \text{ for const vol. process}$$



$$\frac{V}{PA_0} \cdot \int_{-r_A}^X dX_A \Rightarrow \frac{V}{PA_0}$$



making mole bal. in reactor 2 (CSTR1)

$\frac{V_1}{PA_1} = \frac{V_1}{PA_0} + \text{disappearance by chemical. } -x_1 \text{ ft Accumulation}$

$$\Rightarrow PA_1 = PA_0 + (-r_A) V_1$$

$$\Rightarrow PA_1 = PA_2 + V_1 \Rightarrow \frac{(PA_0 - PA_0 x_1)}{(-r_A)} = \frac{(PA_0 - PA_0 x_2)}{(-r_A)}$$

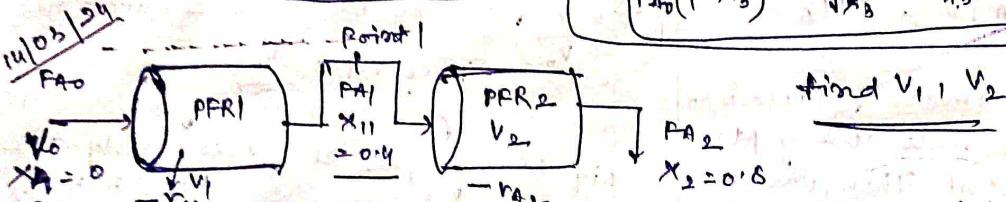
$$\frac{PA_0 (x_2 - x_1)}{(-r_A)} = V_1$$

$$\text{Similarly } \frac{PA_0 (x_3 - x_2)}{(-r_A)} = V_2$$

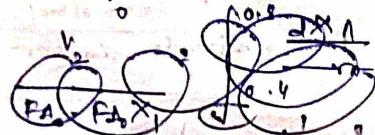
Now, calc. for PBR (reactor 4):

$$\Rightarrow \frac{W}{PA_3} \cdot \int_{x_3}^{x_4} \frac{dX_A}{PA_3} \Rightarrow \frac{W}{PA_0 - PA_0 x_3} = \int_{x_3}^{x_4} \frac{dX_A}{PA_0 - PA_0 x_3}$$

$$\Rightarrow \frac{W}{PA_0 (1-x_3)} = \frac{\int_{x_3}^{x_4} dX_A}{PA_0 - PA_0 x_3}$$



$$\frac{V_1}{PA_0} \int_{-r_A}^{x_1} dX_A = \int_{-r_A}^{0.4} dX_A \Rightarrow \frac{V_1}{PA_1} = \int_{-r_A}^{x_2} \frac{dX_A}{PA_1} = \int_{-r_A}^{0.8} \frac{dX_A}{PA_1}$$



$$\frac{V_1}{PA_0} = \int_{-r_A}^{0.4} dX_A + \int_{-r_A}^{0.8} dX_A$$

$$\rightarrow \frac{V_1}{PA_0} = \int_0^{0.8} \frac{dx}{-r_A}$$

as we already know that $\int_a^b f(x) dx = \int_0^a f(x) dx + \int_a^b f(x) dx$

Design Eqⁿ of a Batch reactor:-

We know that for a batch reactor [inflow = outflow = 0]

$$\frac{dN_A}{dt} = (r_A)V$$

$$\Rightarrow \frac{1}{V} \frac{dN_A}{dt} = r_A$$

$$\Rightarrow -\frac{dCA}{dt} = -r_A$$

$$= k C_A^2$$

$$\rightarrow \int -\frac{dCA}{CA^2} = \int k dt$$

- ① A \rightarrow B (liq. phase)
- ② const. Mol. process
- ③ $-x^n$ follows 2^n order kinetics

Time reqd. to reduce initial conc. (C_{A0}) to a particular conc. at time t

$$\frac{1}{k} \left[\frac{1}{CA} - \frac{1}{CA_0} \right] = t$$

Total time required: $t_t = t_c + t_p + t_e + t_f$

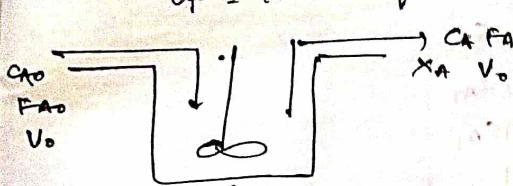
where, t_t = total time required

t_c = time required to charge a feed.

t_p = time required for emptying the reactor

t_e = time req. for cleaning the reactor part $\rightarrow x^n$

t_f = time req. to fill the reactor



x^n follows 1st order kinetics.

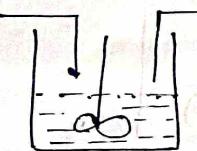
$$\frac{V}{V_0} = \frac{X_A}{(-r_A)_{\text{exit}}} \Rightarrow V = F_{A0} X_A \rightarrow V = V_0 C_{A0} X_A \quad \frac{(-r_A)_{\text{exit}}}{(-r_A)_{\text{exit}}}$$

$$\Rightarrow \left(\frac{V}{V_0} \right) \cdot \frac{C_{A0} X_A}{K_C A} \quad \text{[considering 1st order kinetics]}$$

$$\Rightarrow T = \frac{C_{A0} X_A}{K_C A_0 (1 - X_A)} \rightarrow T K = \frac{X_A}{1 - X_A} \rightarrow T K = \frac{X_A}{X_A}$$

$$\Rightarrow X_A (1 + T K) = T K \rightarrow X_A = \frac{T K}{1 + T K}$$

(183) 24



reaction: $A \xrightarrow{k} R$

let V be the Vol. of CSTR

The x^n follows 1st order kinetics.

from performance eq's we... $(-r_A = k_C A)$

know: $V = F_{A0} X_A$

$$\Rightarrow V = \frac{V_0 C_{A0} X_A}{(-r_A)_{\text{exit}}} \Rightarrow \frac{V}{V_0} = \frac{C_{A0} X_A}{K_C A} \quad \left\{ \frac{V}{V_0} = T \right\}$$

$$\Rightarrow T = \frac{C_{A0} X_A}{K_C A_0 (1 - X_A)} \Rightarrow T K = \frac{X_A}{1 - X_A} \Rightarrow X_A = \frac{T K}{(1 + T K)}$$

relationship b/w fraction conversion & Damkohler no. for a first order rxn

$$C_A = \frac{C_{A0}}{1 + T K} \Rightarrow C_A = \frac{C_{A0}}{1 + D_a}$$

$$\therefore X_A = \frac{D_a}{1 + D_a} \quad C_A \text{ as a fn of } T K \text{ for a first order reaction}$$

Damkohler no. (D_a) = $-r_{A0} V = \text{rxn rate at the entrance condn}$

significance \rightarrow extent of conversion that can be achieved in a CSTR

continuous flow reactor

$$D_a = \frac{F_{A0}}{V_0 C_{A0}} \frac{K C_{A0}^n V}{C_{A0}^{n-1}} = K \left(\frac{V}{V_0} \right)^{n-1} = K T C_{A0}^{n-1} \quad [\text{for a } n^{\text{th}} \text{ order rxn}]$$

Now, for first order rxn $D_a = K T$

for 2nd order rxn $D_a = T K C_{A0}$

$D_a < 0.1 \rightarrow$ less than 10% conversion can be achieved in a CSTR.

$D_a > 10 \rightarrow$ more than 90% conversion can be achieved in a CSTR.

$T K$: Damkohler no./Vessel dispersion no.

$$D_a = \frac{T K}{V_0 C_{A0}} \quad \begin{aligned} & r_{A0} = \text{initial rxn rate} \\ & V = \text{vol. of reactor} \\ & F_{A0} = \text{initial molar flow rate (mole/time)} \end{aligned}$$

$\Rightarrow K C_{A0} V = T K \quad \text{first order}$

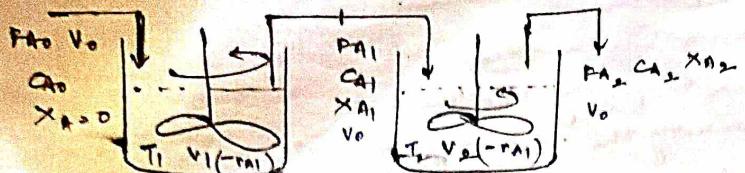
$$\text{for } n^{\text{th}} \text{ order: } -r_{A0}^n V = K C_{A0}^n V = K \left(\frac{V}{V_0} \right)^{n-1} C_{A0} \quad \begin{aligned} & \text{order: } \frac{F_{A0}}{V_0} \\ & \Rightarrow T K C_{A0}^{n-1} \quad \text{rxn} \end{aligned}$$

Physical significance of Damkohler no.: —

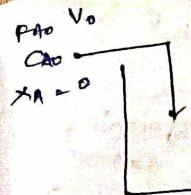
extent of conversion that can be achieved in a CSTR

$$0.1 < D_a < 10$$

the
particulars



- ① $V_1 \neq V_2$
- ② first order kinetics
- ③ V_0 to remain constant



First reactor: $-FA_0 = FA_1 + (-r_A) V_1$

$$\Rightarrow \frac{FA_0 - FA_1}{(-r_A)} = V_1$$

$$\Rightarrow \frac{V_0 CA_0 - V_1 CA_1}{(-r_A)} = V_1$$

$$\Rightarrow \frac{CA_0 - CA_1}{K_1 CA_1} = \frac{V_1}{V_0} = T_1$$

$$\Rightarrow CA_0 - CA_1 = V_1 = T_1$$

$$\Rightarrow CA_0 = CA_1 + T_1$$

$$\Rightarrow CA_0 = CA_1 + T_1 K_1 CA_1$$

$$\Rightarrow CA_0 = (1 + T_1 K_1) CA_1$$

$$\Rightarrow CA_0 = (1 + T_1 K_1) CA_1$$

$$\Rightarrow CA_1 = \frac{CA_0}{1 + T_1 K_1}$$

for 2nd reactor: $-FA_1 = FA_2 + (-r_A) V_2$

$$\Rightarrow \frac{FA_1 - FA_2}{(-r_A)} = V_2$$

$$\Rightarrow \frac{V_0 CA_1 - V_2 CA_2}{(-r_A)} = V_2$$

$$\Rightarrow \frac{CA_1 - CA_2}{K_2 CA_2} = \frac{V_2}{V_0} = T_2$$

$$\Rightarrow CA_1 - CA_2 = K_2 T_2$$

$$\Rightarrow CA_1 = T_2 K_2 CA_2 + CA_2$$

$$\Rightarrow CA_2 = \frac{CA_1}{(1 + T_2 K_2)}$$

$$\Rightarrow CA_2 = \frac{CA_0}{(1 + T_1 K_1)(1 + T_2 K_2)}$$

$$\Rightarrow -r_A = \frac{K_2 CA_0}{(1 + T_1 K_1)(1 + T_2 K_2)}$$

$$CA_n = CA_0$$

$$\frac{(1 + T_1 K_1)}{(1 + T_2 K_2)} \cdots \frac{(1 + T_n K_n)}{(1 + T_K K_K)} = \frac{CA_0}{(1 + T_K K_K)}$$

$$\Rightarrow -r_A = K CA_n = K C_0^n$$

$$X_n = 1 - \frac{1}{(1 + D_A)^n}$$

{ for first order
then $T_K = D_A$ }

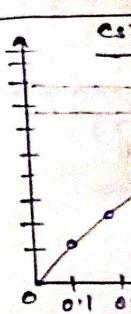
$$T_1 = T_2 = T = \text{if } V_1 = V_2 \text{ are same}$$

$$V_0 \text{ is fixed}$$

$$K_1 = K_2 = K \text{ remain constant}$$

$$-r_A = \frac{K_2 C_0}{(1 + T K)^2}$$

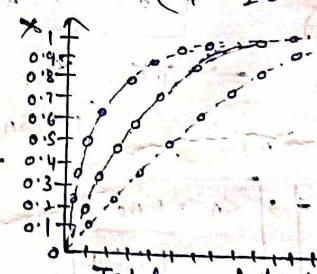
$$X_n = 1 - \frac{1}{(1 + D_A)^2}$$



$$PFR \text{ (series)} = \frac{C_0}{C_n}$$

$$\Rightarrow \frac{T}{C_0} =$$

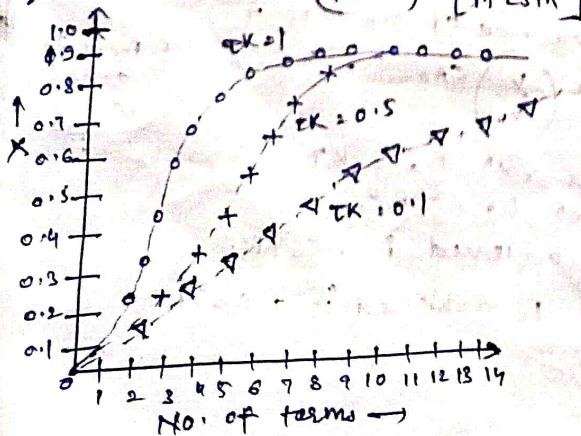
$$\Rightarrow T = \frac{C_0}{K}$$



Total no. of tanks put in series

significance \rightarrow [High T_K value means large reactor vol. & large "x" rate for a const. volumetric flow rate]

A high T_K , only 2-8 tanks are sufficient enough to achieve above 90% of conversion
At low T_K values, we need large no. of tanks in series to achieve above 90% of conversion.

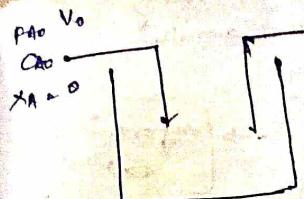


Multiples

- ① Parallel
- ② Series
- ③ CSTR

- ④ Liquid Step 1: CH_3Cl

Step 2:



$$F_A V_0 \rightarrow C_{AO}$$

$$X_A = X_{AP}$$

$$\tau K C_{AO} = \frac{X_A}{(1-X_A)^2} \quad \text{for a 2nd order rxn}$$

$$D_a = \tau K C_{AO}$$

$$\Rightarrow D_a = \frac{X_A}{X_A^2 - 2X_A + 1} \rightarrow D_a X_A^2 - 2D_a X_A + D_a = X_A$$

$$\Rightarrow D_a X_A^2 + (1+2D_a) X_A + D_a = 0$$

$$X_A = \frac{(1+2D_a) \pm \sqrt{(1+2D_a)^2 - 4D_a}}{2D_a}$$

$$X_A = \frac{(1+2D_a) \pm \sqrt{1+4D_a + 4D_a^2 - 4D_a}}{2D_a}$$

$X_A = 1$ {In reversible rxn}
 $X_A = X_e$ (reversible rxn)

$$X_A = \frac{(1+2D_a) \pm \sqrt{1+4D_a}}{2D_a}$$

For 2nd order kinetics

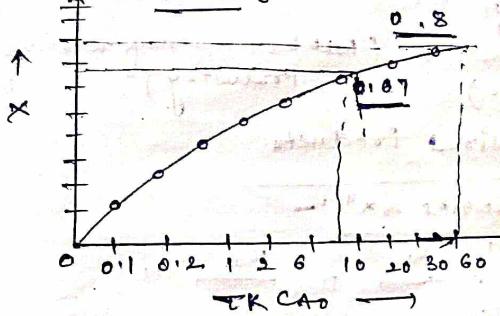
$$V = F_A D_a X_A = V_0 C_{AO} X_A$$

$$(-r_A)|_{\text{exit}} = \frac{V}{V_0} \frac{C_{AO} X_A}{K C_{AO}^2}$$

$$V = \frac{C_{AO} X_A}{K [C_{AO}(1-X_A)^2]}$$

$$\Rightarrow \tau K = \frac{X_A}{C_{AO}(1-X_A)^2}$$

CSTR (V_0 is const.)



PFR (second order kinetics)

const. density system.

$$V = F_A D_a \int \frac{dx}{x} = V_0 C_{AO} \int \frac{dx}{k C_{AO}^2} \Rightarrow \left(\frac{V}{V_0} \right) \left(\frac{1}{C_{AO}} \right) = \int \frac{x dx}{k C_{AO}^2} \rightarrow T = \int \frac{x dx}{k C_{AO} (1-x)} \quad \text{A}$$

$$\Rightarrow \frac{T}{C_{AO}} = \frac{1}{k C_{AO}^2} \int \frac{x dx}{(1-x)^2}$$

$$\Rightarrow \frac{\tau K C_{AO}}{V_0} = \frac{1}{k} \int \frac{x dx}{(1-x)^2} = \left[\frac{(1-x)^{-1}}{-1} \right]_0^x = 1 - \frac{1}{1-x}$$

$$\Rightarrow \tau K C_{AO} = \frac{x}{1-x}$$

$$\Rightarrow X = \frac{D_a}{1+D_a} \quad [D_a = \frac{x}{\tau K C_{AO}}]$$

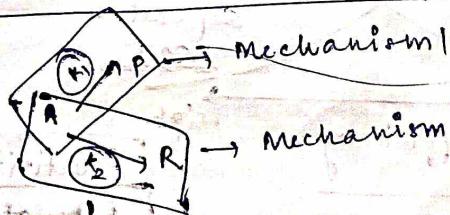
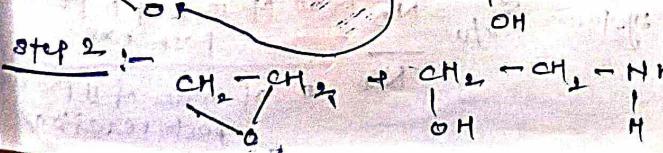
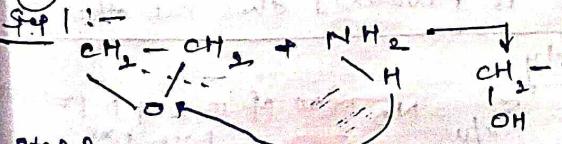
Multiple reactions! :-

i) Parallel rxn

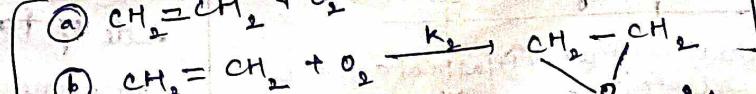
ii) Series rxn

iii) complex rxn → (parallel + series)

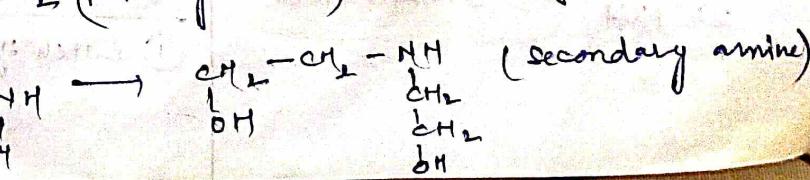
iv) independent rxn → petroleum refinery

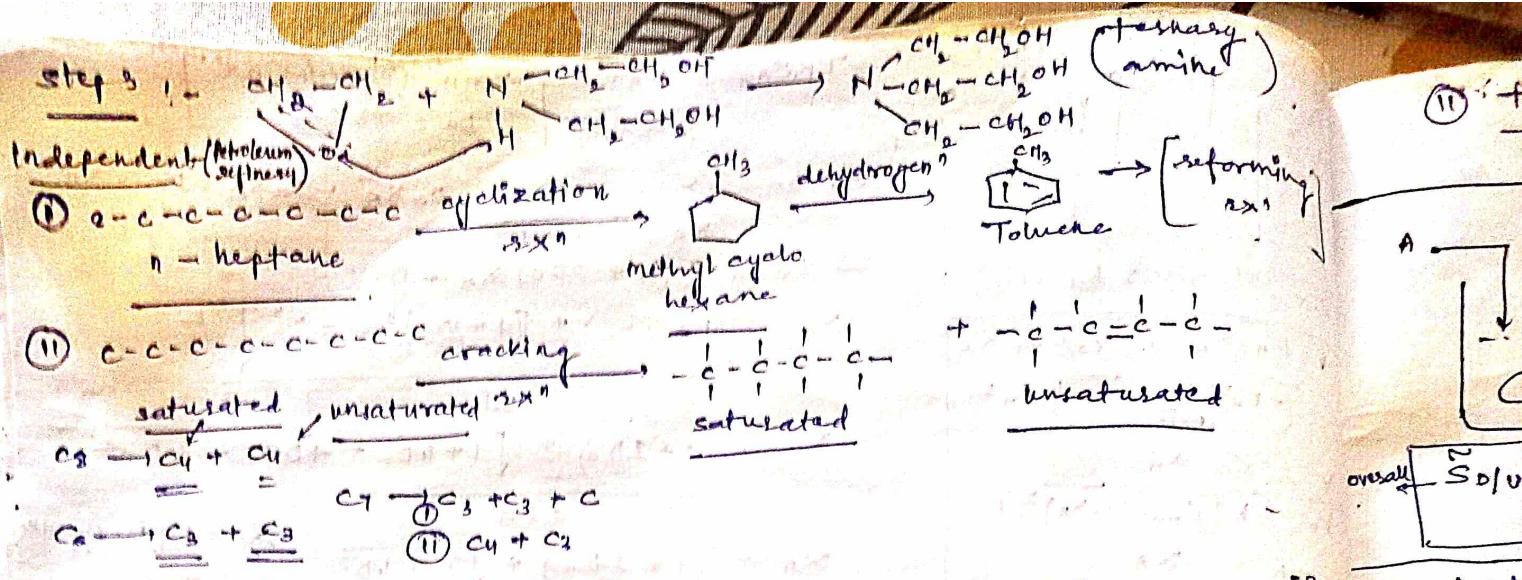


Mechanism 2

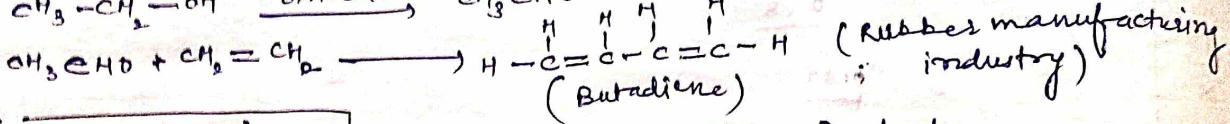
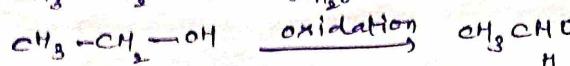
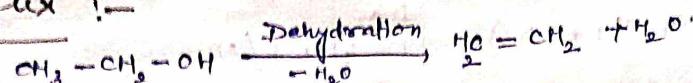


Ethylen oxide





Complex :-



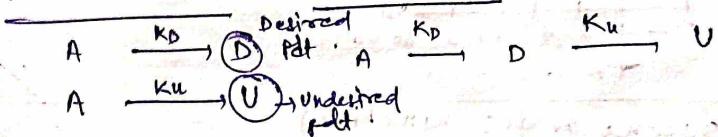
21/2/54

Multiple rxns :-

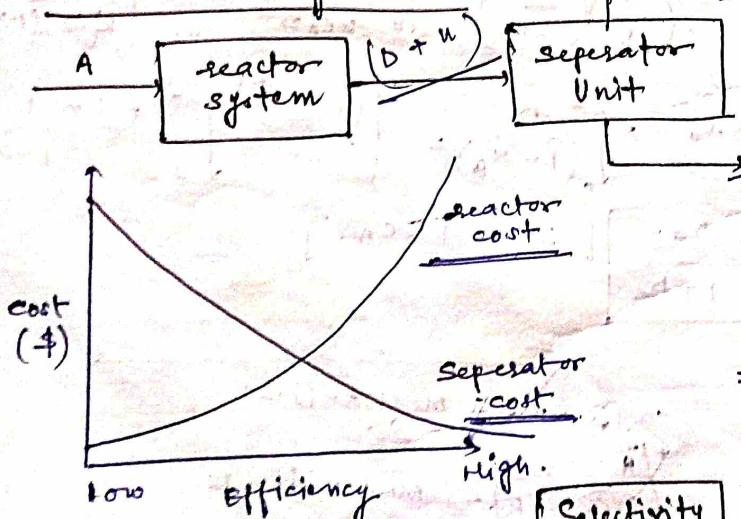
- (I) Parallel rxns
- (II) Series rxns
- (III) Complex rxns
- (IV) Independent rxns

Desired & Undesired Products

parallel rxns :- Series rxn !-



Reactor arrangement :-



Selectivity & Yield :-

- (I) Instantaneous selectivity
- (II) Overall selectivity
- (I) Instantaneous Yield.
- (II) Overall Yield.

Aim \rightarrow our aim would be to maximise the product of desired products and minimise the prod. of undesired pdts.

\rightarrow This can be achieved by 2 ways:-

a) Using raw, expensive & sophisticated reactor system \rightarrow this would lower down the prod. of undesired pdt.

or b) We can use an expensive separator unit \rightarrow which would effectively separate the desired and undesired products.

Selectivity

rate of form' of the desired pdt. $\frac{dD}{dt} = S_D \propto S_D/U$

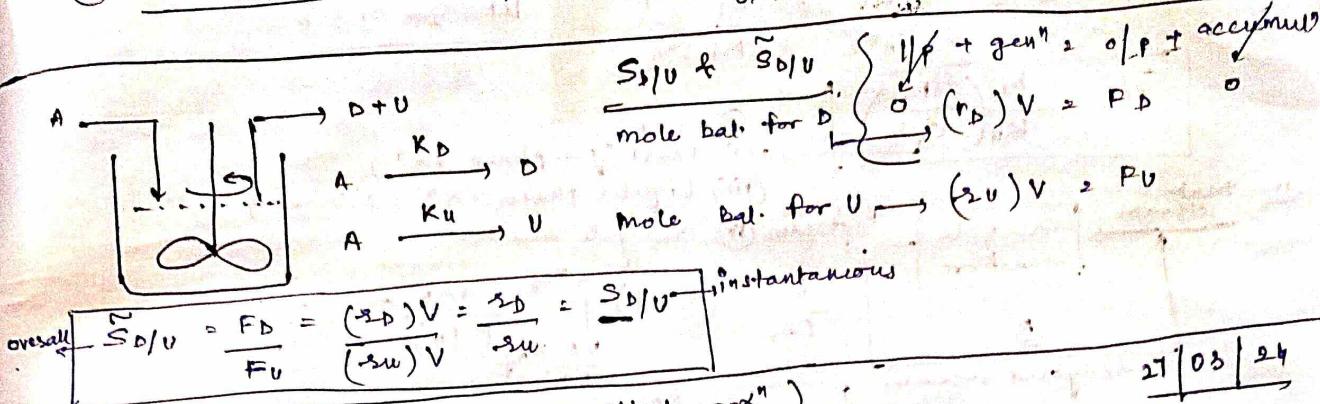
rate of form' of undesired pdt. $\frac{dU}{dt} = S_U \propto S_U/U$ (T.S.)

how one pdt. is favoured over the other one

Overall selectivity

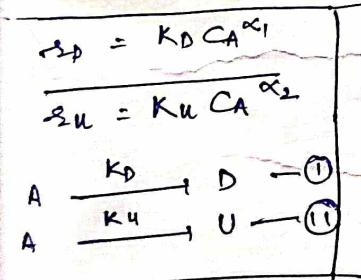
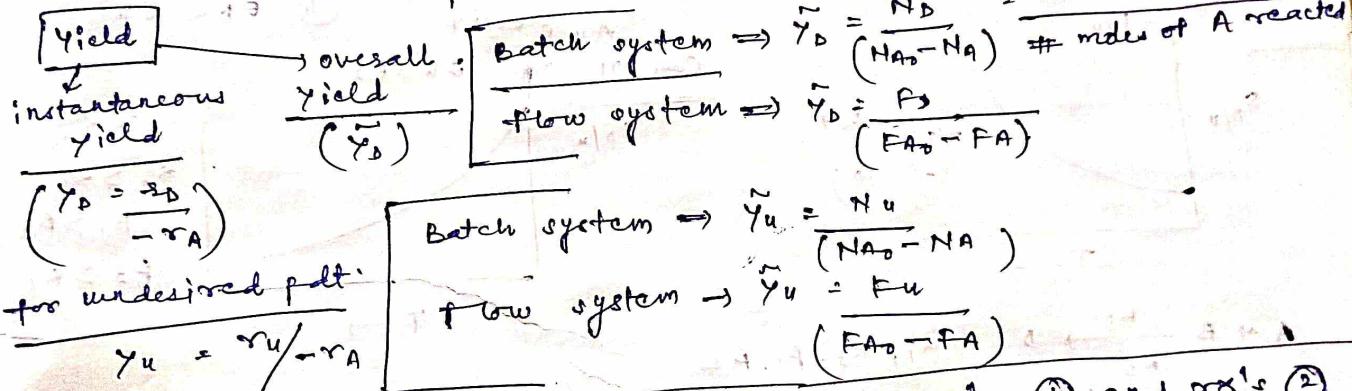
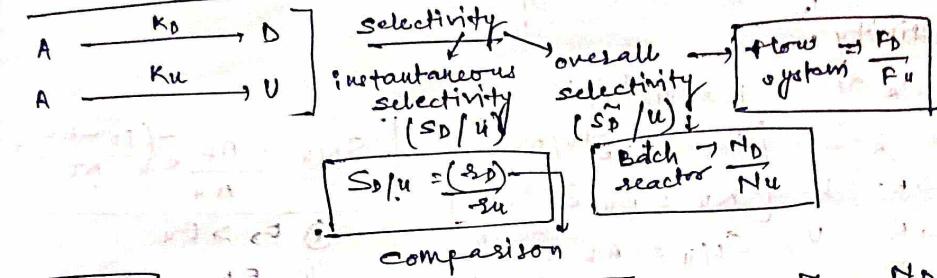
(I) Batch system $S_D/U = N_D/N_U = \frac{\# \text{ of moles of } D \text{ produced post rxn}}{\# \text{ of moles of } U \text{ produced post reaction.}}$

(1) flow system : $\tilde{S}_D/U = \frac{P_D}{P_U}$ exit molar flow rate of desired prod.
 $\tilde{S}_D/U = \frac{P_D}{P_U}$ exit molar flow rate of undesired prod.



27/03/24

Desired & Undesired products (multiple rxn)

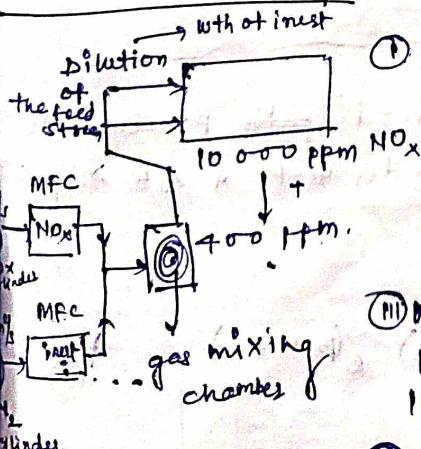


Let α_1, α_2 are the orders of the rxn's (1) and rxn's (2) respectively. α_1 and α_2 are +ve quantity
maximise the productivity of D

$$\tilde{S}_D/U = \frac{r_D}{r_U} = \frac{K_D C_A^{\alpha_1}}{K_U C_A^{\alpha_2}} \Rightarrow \frac{\tilde{S}_D/U}{K_U} = \frac{r_D}{r_U} = \frac{K_D}{K_U} C_A (\alpha_1 - \alpha_2)$$

$$\tilde{S}_D/U \propto C_A$$

$$\tilde{S}_D/U = \left(\frac{K_D}{K_U} \right) C_A^{\alpha}$$



- (i) $\alpha_1 > \alpha_2$ high productivity of D
- (i) Batch reactor/ PFR
- (ii) CSTR's must be avoided, (perfectly mixed, no conc of D)

- (iii) We use inlet gas for dilution bcoz otherwise we will have some byproduct gases. (400 ppm + H₂/CO₂/CO)
feed conc should be maintained at the min. value \rightarrow feed stream shouldn't be diluted
- (iv) Diluent should be avoided.
- (v) high P \rightarrow CA

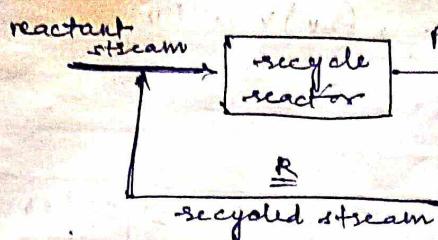
(iii) $\alpha_1 < \alpha_2$



$$S_D/u = \frac{\gamma_D}{\gamma_u} = \frac{K_D C_A^{\alpha_1}}{K_u C_A^{\alpha_2}} = \frac{K_D}{K_u} \frac{1}{C_A (\alpha_2 - \alpha_1)} \quad \text{but } \alpha_2 - \alpha_1 > 0$$

$$S_D/u = \frac{K_D}{K_u} \left(\frac{1}{C_A b} \right)$$

- ① CSTR
- ② Ideal (gas phase \Rightarrow)
- ③ Liquid phase \Rightarrow (Diluent)
- ④ Recycle reactor



$$\frac{V}{F_A u} = (R+1) \int_{\frac{P_A}{P_A u}}^{\frac{P_A}{P_A u}} \frac{dx_A}{\frac{R}{R+1} x_A} \rightarrow x_A$$

$$\frac{V}{F_A u} = \int_0^{x_A} \frac{dx_A}{(\frac{R}{R+1})}$$

Effect of T on Selectivity :-

$$S_D/u = \frac{\gamma_D}{\gamma_u} = \frac{K_D C_A^{\alpha_1}}{K_u C_A^{\alpha_2}} \quad K_D = A_D e^{-E_D/RT}$$

$$\frac{S_D/u}{K_D} \leftarrow R \dots D$$

$$\begin{cases} K_D = A_D e^{-E_D/RT} \\ K_u = A_u e^{-E_u/RT} \end{cases}$$

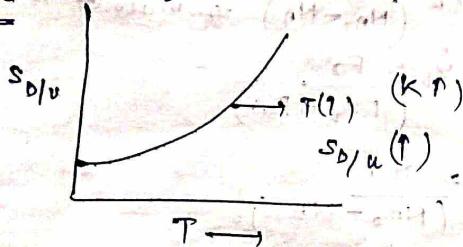
$$S_D/u = A_D e^{-E_D/RT}$$

$$S_D/u = \frac{A_D}{A_u} e^{-\left(\frac{E_D - E_u}{RT}\right)}$$

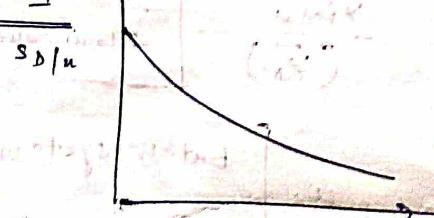
i) $E_D > E_u$

ii) $E_D < E_u$

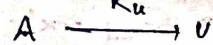
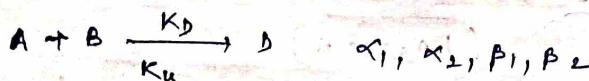
Case I, $E_D > E_u$



Case II



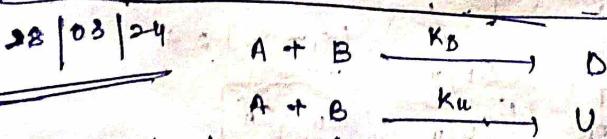
$$\begin{cases} \alpha_1 > \alpha_2 \\ \alpha_2 > \alpha_1 \\ \beta_1 > \beta_2 \\ \beta_2 > \beta_1 \end{cases}$$



$$\frac{\gamma_D}{\gamma_u} = \frac{\gamma_D}{\gamma_u} = \frac{K_D}{K_u} \frac{C_A (\alpha_1 - \alpha_2)}{C_B (\beta_1 - \beta_2)}$$

$$\gamma_D = K_D C_A^{\alpha_1} C_B^{\beta_1}$$

$$\gamma_u = K_u C_A^{\alpha_2} C_B^{\beta_2}$$



We need to maximize the productivity of the desired path production (D)

$$\gamma_D = K_D C_A^{\alpha_1} C_B^{\beta_1}$$

($\alpha_1, \beta_1, \alpha_2, \beta_2$ are the order w.r.t A & B respectively)

$$\gamma_u = K_u C_A^{\alpha_2} C_B^{\beta_2}$$

$$\gamma_A = \gamma_D + \gamma_u = (K_D C_A^{\alpha_1} C_B^{\beta_1} + K_u C_A^{\alpha_2} C_B^{\beta_2})$$

$$S_D/u = \frac{\gamma_D}{\gamma_u} = \frac{K_D C_A^{\alpha_1} C_B^{\beta_1}}{K_u C_A^{\alpha_2} C_B^{\beta_2}} = \left(\frac{K_D}{K_u} \right) C_A^{\alpha_1 - \alpha_2} C_B^{\beta_1 - \beta_2}$$

Case I :- $\alpha_1 > \alpha_2 ; \beta_1 > \beta_2$

$$\Rightarrow (\alpha_1 - \alpha_2) = +ve = a$$

$$\text{and } \beta_1 > \beta_2 \Rightarrow (\beta_1 - \beta_2) = +ve = b$$

Now, eqn (1) can be written as

$$S_D/u = \frac{K_D C_A^\alpha C_B^\beta}{K_u}$$

Case II :- $\alpha_1 > \alpha_2 ; \beta_1 < \beta_2$

Case III :- $\alpha_1 < \alpha_2 ; \beta_1 < \beta_2$

Case IV :- $\alpha_1 < \alpha_2 ; \beta_2 > \beta_1$

If we want to maximize the productivity of D, both C_A & C_B should be high.

- # Possibility →
 - I Batch / PFR
 - II High Fr. (A as phase rx's)
 - III CSTR should be avoided.
 - IV We should not use diluent / inert.

Case II :- $\alpha_1 > \alpha_2 ; \beta_1 < \beta_2$

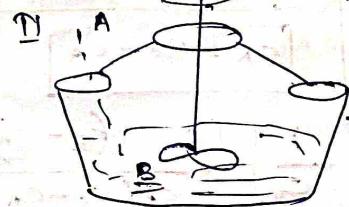
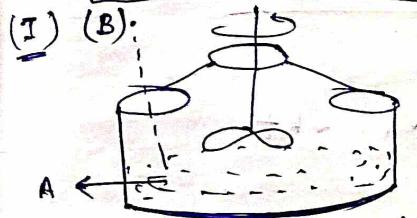
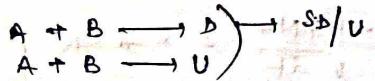
$$\Rightarrow (\alpha_1 - \alpha_2) = +ve \text{ quantity} = a$$

$$\beta_1 < \beta_2 \Rightarrow \beta_2 - \beta_1 = +ve = b$$

$$S_D/u = \frac{K_D C_A^{\alpha_1 - \alpha_2}}{K_u} = \frac{K_D \left(\frac{C_A^a}{C_B^b} \right)}{K_u}$$

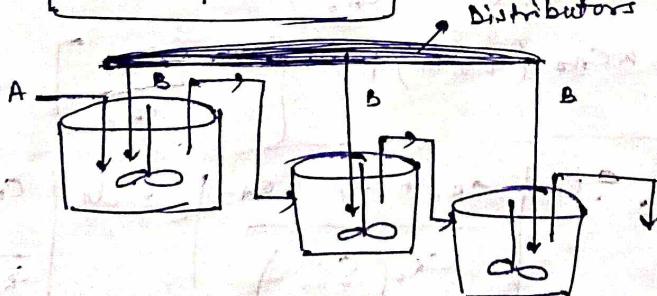
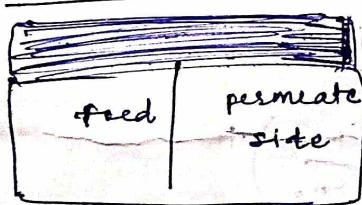
Semi batch reactor with arrangement I.
II Membrane reactor

Semi batch reactor (generally used for liquid phase rx's)



A already present & we are dropping B in a dropwise manner
B present already & we are adding A in dropwise manner

membrane reactor → selectively allows some of the feed to go to the permeate side.



Case III

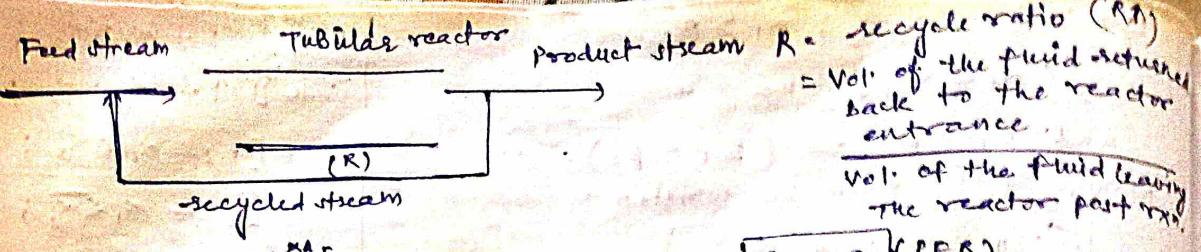
$$S_D/u = \frac{K_D C_A^{\alpha_1 - \alpha_2} C_B^{\beta_1 - \beta_2}}{K_u}$$

$$S_D/u = \frac{1}{K_u C_A C_B}$$

$$C_A(t) \quad C_B(t) \rightarrow S_D/u \uparrow$$

Arrangements :-

- I CSTR
- II use more diluents / inert
- III Low pressure (for a gas phase rx')
- IV Tubular reactor with high recycle ratio.



$R = \text{recycle ratio}$ (R)
 $= \text{Vol. of the fluid returned back to the reactor entrance.}$

$\text{Vol. of the fluid leaving the reactor part}$ (x_A)

$$R = O - f PFR$$

$$R = L - f MFR \rightarrow \text{Mixed flow rate}$$

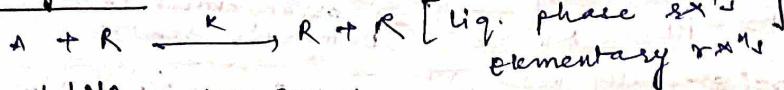
$$\text{Case IV: } S_D/u = \frac{K_D}{K_u} \frac{C_A^{\alpha_1 - \alpha_2} C_B^{\beta_1 - \beta_2}}{C_A^\alpha}$$

arrangements :- ① Semibatch reactor with arrangement ①

② Membrane reactor

③ CSTR's in series with A fed to each reactor

Autocatalytic ex^n :



$$-r_A = -\frac{1}{V} \frac{dN_A}{dt} = k C_A C_R$$

$$-r_A = -\frac{dC_A}{dt} = k C_A C_R$$

$$\frac{dC_A}{C_A(C_0 - C_A)} = -k dt \Rightarrow \frac{1}{C_0} \int \frac{[C_A + (C_0 - C_A)]}{C_A(C_0 - C_A)} dC_A = -kt.$$

$$\Rightarrow \frac{1}{C_0} \int \frac{C_A dC_A}{C_A(C_0 - C_A)} + \frac{1}{C_0} \int \frac{(C_0 - C_A) dC_A}{C_A(C_0 - C_A)} = -kt$$

$$\Rightarrow \left[-\ln(C_0 - C_A) \right]_{C_0}^{C_A} + \left[\ln C_A \right]_{C_0}^{C_A} = -k C_0 t$$

$$\Rightarrow \ln \left| \frac{C_A}{C_0} \left[\frac{C_0 - C_{A_0}}{C_0 - C_A} \right] \right| = -k(C_{A_0} + C_{R_0})t$$

$$\ln \left| \frac{C_A}{C_0} \left[\frac{C_0 - C_{A_0}}{C_0 - C_A} \right] \right| = -k C_{A_0} \left(1 + \frac{C_{R_0}}{C_{A_0}} \right) t$$

$$\textcircled{a} \quad \ln \left| \frac{M \cdot x_A}{M(1 - x_A)} \right| = -k C_{A_0} (1 + M) t \quad [M = \frac{C_{R_0}}{C_{A_0}}]$$

$$\Rightarrow \ln \left| \frac{\frac{C_{R_0}}{C_{A_0}} + \left(1 - \frac{C_A}{C_{A_0}} \right)}{\frac{C_{R_0}}{C_{A_0}} \left(\frac{C_A}{C_{A_0}} \right)} \right| = \ln \left| \frac{C_{R_0} + C_{A_0} - C_A}{C_{R_0} \left(\frac{C_A}{C_{A_0}} \right)} \right| = \ln \left| \frac{C_{R_0} \left(\frac{C_A}{C_{A_0}} \right)}{C_{R_0} + C_{A_0}} \right|$$

$$= -\ln \left| \frac{C_A (C_0 - C_{A_0})}{C_{A_0} (C_0 - C_A)} \right|$$

Semi batch

A + B -

A + B -

- $S_D =$

$S_M =$

S_D/u

To imp
CA & CR
should
mole b

$\frac{N_A}{V}$

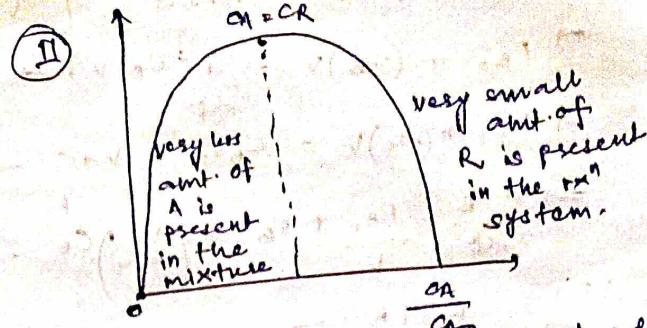
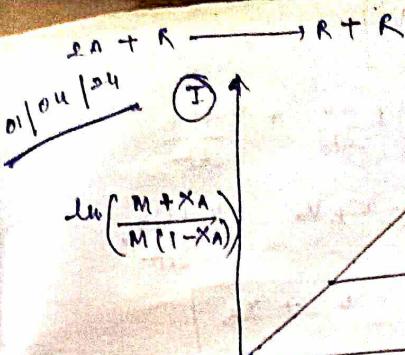
① ex
② $\frac{M}{M}$
③ over

reactant A
balance

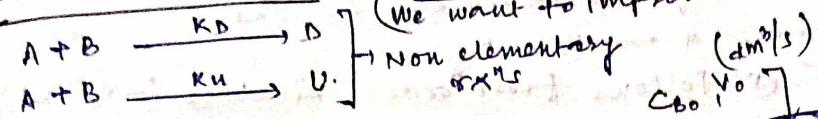
\Rightarrow

reactant B

for B



Semi batch reactor : — Lq. phase rxn



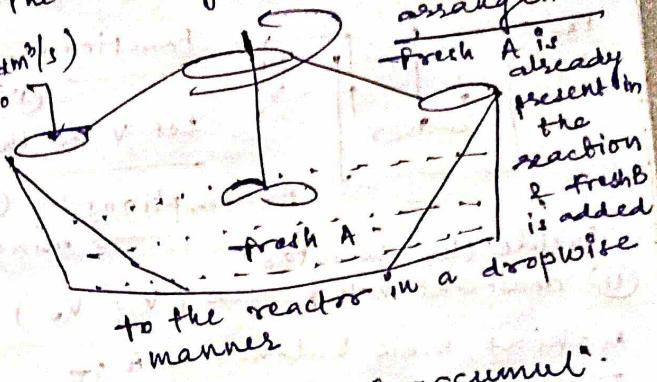
$$S_D/U = K_D C_A^2 C_B$$

$$S_{DU} = K_u C_A C_B^2$$

$$S_D/U = \frac{r_D}{r_u} = \left(\frac{K_D}{K_u} \right) \left(\frac{C_A}{C_B} \right)$$

To improve the selectivity of D
CA should be high & CB
should be low.

$$\text{mole balance eqn} : - \frac{1/p - o/p}{o - o} = \text{disappearance rate of accumulated}$$



to the reactor in a dropwise manner

$$\frac{dN_A}{dt} = r_A V(t)$$

$$\frac{N_A}{V} = C_A \Rightarrow N_A = C_A V$$

$$r_A V(t) = \frac{d(C_A V)}{dt}$$

$$r_A V(t) = V \frac{dC_A}{dt} + C_A \frac{dV}{dt}$$

- ① concentration
- ② # of moles
- ③ conversion

variables in
semi batch
reactor.

overall species balance :-

$$\rho_0 V_0 = \frac{d(pV)}{dt} \rightarrow \rho_0 V_0 = p \frac{dV}{dt} \rightarrow \frac{dV}{dt} = V_0$$

cont. density process ($\rho_0 = \rho$)

$$\text{reactant balance} \Rightarrow r_A \frac{V(t)}{V_0} = \frac{V}{V_0} \frac{dC_A}{dt} + C_A \Rightarrow r_A \frac{V(t)}{V_0} - C_A = \frac{V}{V_0} \frac{dC_A}{dt}$$

$$\Rightarrow r_A \frac{V(t)}{V} - \frac{V_0 C_A}{V} = \frac{dC_A}{dt}$$

$$\frac{r_A - V_0 C_A}{V} = \frac{dC_A}{dt}$$

$$\text{reactant B} : - \int_{V_0}^V dV = V_0 \int_0^t dt \rightarrow V - V_0 = V_0 t \rightarrow V = V_0 + V_0 t = V_0 (1 + t)$$

$$\text{for B} : - \frac{1/p - o/p}{o - o} = \text{disappearance by chemical rxn} + \text{accumulation}$$

reactant A

volumetric
feed flow rate
of B.

$$\Rightarrow P_{B_0} = -(r_B)V(t) + \frac{dN_B}{dt}, \quad \left[\frac{N_B}{V} = C_B \rightarrow N_B = C_B V \right]$$

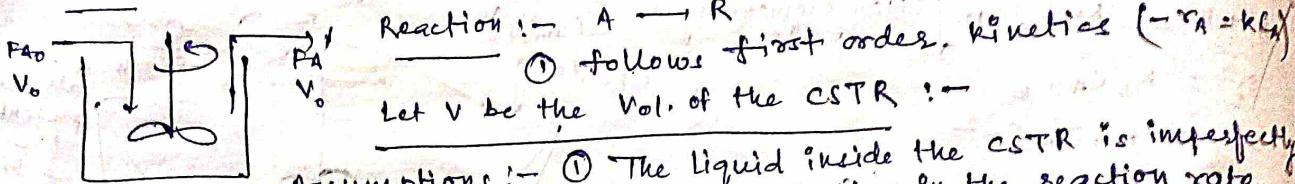
$$\Rightarrow P_{B_0} + (r_B)V = \frac{d(C_B V)}{dt} \rightarrow P_{B_0} + (r_B)V = C_B \frac{dV}{dt} + V \frac{dC_B}{dt}$$

$$\Rightarrow P_{B_0} + (r_B)V = C_B V_0 + V \frac{dC_B}{dt} \rightarrow P_{B_0} + (r_B)V - C_B V_0 = V \frac{dC_B}{dt}$$

$$\Rightarrow \frac{dC_B}{dt} = \frac{P_{B_0}}{V} + r_B - \left(\frac{V_0}{V} \right) C_B \rightarrow \boxed{\frac{dC_B}{dt} = \frac{P_{B_0} - V_0 C_B}{V} + r_B}$$

3/04/24. CSTR :-

Aim:- To obtain the time required to achieve ss cond'.



Assumptions:- ① The liquid inside the CSTR is imperfectly mixed \rightarrow No variation in the reaction rate

inside the reactor

(ii) constant vol. process ($V = V_0$)

Making mole balance on A :-

$$[\text{O/P}] - [\text{O/I}] = \text{Disappearance by chemical rxn} + \text{rate of accumulation} \Rightarrow P_{AO} - P_A - (kCA)V = \frac{dNA}{dt}$$

$$\Rightarrow V_0 C_{AO} - V_0 C_A - kCAV = \frac{d[C_A V]}{dt} \Rightarrow V_0 C_{AO} - V_0 C_A - kCAV = V \frac{dC_A}{dt} \quad \left[\frac{dV}{dt} = 0 \right]$$

$$\Rightarrow C_{AO} - C_A - \frac{kCAV}{V_0} = \frac{V}{V_0} \frac{dC_A}{dt} \Rightarrow C_{AO} - C_A - kT\ln \frac{C_A}{C_{AO}} = \frac{V}{V_0} \frac{dC_A}{dt} \Rightarrow C_{AO} = C_A + \frac{V}{V_0} \frac{dC_A}{dt} + (1+TK)$$

$$\boxed{\frac{C_{AO}}{V} = \frac{dC_A}{dt} + \left(\frac{1+TK}{V} \right) C_A}$$

$$\frac{dy}{dx} + py = q \Rightarrow \text{IF} = e^{\int pdx} \\ \int pdx \Rightarrow \frac{d}{dx} \left[y e^{\int pdx} \right] = \int q e^{\int pdx} dx + c$$

$$\frac{dy}{dx} e^{\int pdx} + p e^{\int pdx} y = q e^{\int pdx}$$

$$\Rightarrow y e^{\int pdx} = \int q e^{\int pdx} dx + c$$

$$p = \frac{1+TK}{V} = \frac{C_{AO}}{V}$$

$$\frac{dC_A}{dt} e^{\int \frac{(1+TK)}{V} dt} + \left(\frac{1+TK}{V} \right) C_A e^{\int \frac{(1+TK)}{V} dt} = C_{AO} e^{\int \frac{(1+TK)}{V} dt}$$

$$\Rightarrow \frac{dC_A}{dt} e^{\int \frac{(1+TK)}{V} dt} = \int \frac{C_{AO}}{V} e^{\int \frac{(1+TK)}{V} dt} dt + c$$

$$\Rightarrow C_A e^{\int \frac{(1+TK)}{V} dt} = \frac{C_{AO}}{V} e^{\int \frac{(1+TK)}{V} dt} \left(\frac{V}{1+TK} \right) + c$$

$$\Rightarrow C_A e^{\int \frac{(1+TK)}{V} dt} = \frac{C_{AO}}{V} e^{\int \frac{(1+TK)}{V} dt} + c \Rightarrow c = \frac{-C_{AO}}{1+TK}$$

initial cond':- at $t = 0$, $C_A = 0$ (reactor cond')

$$C_A e^{\int \frac{(1+TK)}{V} dt} = \frac{C_{AO}}{1+TK} \exp \left(\frac{(1+TK)}{V} t \right) - \frac{C_{AO}}{1+TK}$$

$$\Rightarrow C_A e^{\left(\frac{(1+TK)}{T}\right)t_s} = \frac{C_{A0}}{1+TK} \left[e^{\left(\frac{(1+TK)}{T}\right)t_s} - 1 \right] \Rightarrow C_A = \frac{C_{A0}}{1+TK} \left[1 - e^{-\left(\frac{(1+TK)}{T}\right)t_s} \right]$$

Let us assume that t_s be the time required to obtain 99% of the SS conc (C_A)

$$C_A = \frac{C_{A0}}{1+TK} \quad [C_A = 0.99 C_{A0}]$$

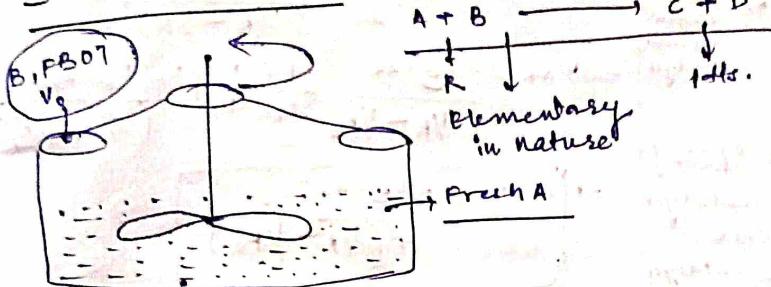
$$C_A = C_{A0} \left[1 - e^{-\left(\frac{(1+TK)}{T}\right)t_s} \right] \Rightarrow 0.99 = 1 - e^{-\left(\frac{(1+TK)}{T}\right)t_s}$$

$$\Rightarrow \left(1 + \frac{TK}{T}\right)t_s = 7.6 \rightarrow t_s = \frac{7.6 T}{1 + TK}$$

cond' 1 :- rxn is rapid. $\Rightarrow TK \gg 1 \rightarrow t_s = \frac{7.6 T}{TK} = \frac{7.6}{K}$

cond' 2 :- rxn is slow $\Rightarrow 1 \gg TK \rightarrow t_s = 7.6 T$

Semibatch reactor:-



$$\text{I} \quad \frac{dC_A}{dt} = -k_{CA} C_A - \frac{V_0}{V}$$

derived in class.

$$\text{II} \quad \frac{dC_B}{dt} = -k_{CA} C_A \frac{V_0}{V}$$

$$\text{III} \quad \frac{dC_C}{dt} =$$

$$\text{IV} \quad \frac{dC_D}{dt} =$$

mole bal on C :- rate of gen' of C = rate of accumul' of C $\quad [\text{as inflow} = \text{outflow} = 0]$

$$\Rightarrow (r_C) V(t) = \frac{dN_C}{dt} \quad \left[\frac{N_C}{V} = C_C \right] \Rightarrow r_C V(t) = \frac{d(C_C V)}{dt}$$

$$\Rightarrow r_C V(t) = V \frac{dC_C}{dt} + C_C \frac{dV}{dt} \Rightarrow r_C V(t) = V \frac{dC_C}{dt} + C_C V_0 \quad [\frac{dV}{dt} = V_0]$$

$$\Rightarrow k_{CA} C_A (V) = V \frac{dC_C}{dt} + C_C V_0 \rightarrow K_{CA} C_A = \frac{V_0 C_C}{V} = \frac{dC_C}{dt} \quad \text{Expression for } C$$

Semibatch reactor

$$\frac{dV}{dt} = V_0 \quad \left| \begin{array}{l} \text{at } t=0, V=V_0 \\ \text{at } t=t, V=V \end{array} \right.$$

$$\Rightarrow dV = V_0 dt \rightarrow (V - V_0) = V_0 t$$

$$\Rightarrow V = V_0 + V_0 t$$

$$X = \text{conversion.} = \frac{N_{A0} - N_A}{N_{A0}}$$

$$B_C \quad t=0, V=V_0$$

$$t=t, V=V$$

$$\rightarrow T = T_0 + t \rightarrow dT = dt$$

$$X = \frac{V_0 C_{A0} - V C_A}{V_0 C_{A0}}$$



$$\frac{N_A}{V} = \frac{N_{A0}(1-X)}{V}$$

$$C_A =$$

$$C_B = F_{B0t} - N_{A0} X$$

$$C_C = N_{A0} X / V$$

$$C_D = N_{A0} X / V$$

$$C_A = \frac{N_{A0}(1-X)}{(V_0 + V_0 t)}$$

$$C_B = F_{B0t} - N_{A0} X$$

$$\frac{C_B}{(V_0 + V_0 t)} =$$

$$C_C = \frac{N_{A0} X}{(V_0 + V_0 t)}$$

$$C_D = N_{A0} X$$

$$\frac{C_D}{(V_0 + V_0 t)} =$$

for B :-

Total no. of moles = Total no. of moles of B present of B in the reactor in the reactor at time t (initially)

+ Total no. of moles of B fed to the reactor HU time of B converted upto Hmet

$$N_B = N_{B0} + \int_{0}^{H} F_{B0} dt - N_{A0} X$$

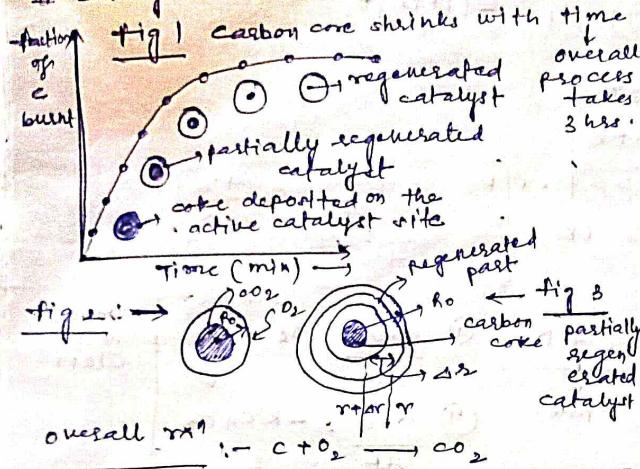
$$N_B = F_{B0t} - N_{A0} X \quad \because N_{C1}, N_{D1} =$$

$$N_C = N_{C1} + N_{A0} X \rightarrow N_{C2} N_{A0} X$$

$$N_D = N_{D1} + N_{A0} X \rightarrow N_D = N_{A0} X$$

8/4/24 - Catalyst regeneration:-

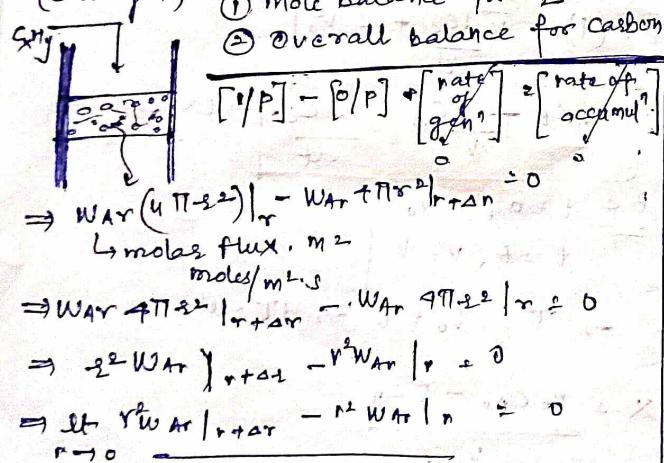
- # catalyst in pellet form.
- # spherical shape of the catalyst
- # catalyst is porous in nature.



[1 mole of O_2 is producing 1 mole of CO_2]

Let R_o be the outer radius of the catalyst
 R be the radius of the carbon core
 $(R_o - R)$ = Regenerated part of the catalyst

Aim: - find out the time required to completely regenerate the surface (catalyst)



$\Rightarrow \frac{d}{dr} \left(r^2 W_{AR} \right) = 0$

$\Rightarrow -D_c \frac{d}{dr} \left(r^2 \frac{dC}{dr} \right) = 0$

$\Rightarrow \frac{d}{dr} \left(r^2 \frac{dC}{dr} \right) = 0$

$\Rightarrow -r^2 \frac{dC}{dr} = K_1$

$\Rightarrow \frac{dC}{dr} = \frac{K_1}{r^2} \Rightarrow \int dC = K_1 \int \frac{dr}{r^2} \Rightarrow C_A = K_1 \left(\frac{-1}{r} \right) + K_2$

$\Rightarrow C_A = -\frac{K_1}{r} + K_2$

$$0 = \frac{-K_1 + K_2}{R} \Rightarrow K_1 = K_2$$

$$CA_0 = K_1 \left(\frac{1}{R} - \frac{1}{R_o} \right)$$

$$K_1 = \frac{CA_0}{\left(\frac{1}{R} - \frac{1}{R_o} \right)}, K_2 = \frac{CA_0}{R \left(\frac{1}{R} - \frac{1}{R_o} \right)}$$

$$CA = \frac{-CA_0}{\left(\frac{1}{R} - \frac{1}{R_o} \right)} + \frac{CA_0}{R \left(\frac{1}{R} - \frac{1}{R_o} \right)} = CA_0 \left[\frac{1}{R \left(\frac{1}{R} - \frac{1}{R_o} \right)} \right]$$

con profile of O_2

$$\Rightarrow \frac{CA}{CA_0} = \frac{\left(\frac{1}{R} - \frac{1}{R_o} \right)}{\left(\frac{1}{R} - \frac{1}{R_o} \right)} = 1$$

$$\Rightarrow W_{AR} = -D_c \frac{d}{dr} \left[\frac{CA_0 \left(\frac{1}{R} - \frac{1}{R_o} \right)}{\left(\frac{1}{R} - \frac{1}{R_o} \right)} \right]$$

$$\Rightarrow W_{AR} = \frac{D_c CA_0}{\left(\frac{1}{R_o} - \frac{1}{R} \right)} \frac{d}{dr} \left(\frac{1}{r} \right) = \frac{D_c CA_0}{\left(\frac{1}{R_o} - \frac{1}{R} \right)}$$

$$\Rightarrow W_{AR} = -\frac{D_c CA_0}{r^2 \left(\frac{1}{R_o} - \frac{1}{R} \right)}$$

Mole balance for Carbon Layer:-

$\frac{dC}{dt} = \text{rate of disappearance of C} + \text{rate of accumulation}$

$$\Rightarrow \frac{dC}{dt} = (-r_c'') + \pi r^2 \frac{dC}{dt} + D_c \phi \frac{4\pi R^2}{3}$$

$$\Rightarrow -r_c'' + \pi r^2 \frac{dC}{dt} = \frac{1}{V} \left(D_c \phi \frac{4\pi R^2}{3} \right)$$

D_c = molar diffusivity of carbon
 ϕ = volume fraction of carbon

$$\Rightarrow -r_c'' + \pi r^2 \frac{dC}{dt} = D_c \phi \frac{4\pi R^2}{3} \frac{dC}{dr}$$

$$\Rightarrow -r_c'' = D_c \phi \frac{dC}{dr} \quad \left[-r_c'' = -W_{AR} \frac{1}{r_o R} \right]$$

$$\Rightarrow -r_c'' = \frac{D_c CA_0}{R^2} \left(\frac{1}{R} - \frac{1}{R_o} \right)$$

$$\Rightarrow -r_c'' = \frac{D_c CA_0}{R^2} \frac{1}{\left(R - R^2/R_o \right)}$$

$$\Rightarrow \int dt = -\frac{D_c \phi}{D_c CA_0} \int \frac{dt}{\left(R - R^2/R_o \right)} \frac{dR}{dR}$$

$$\Rightarrow \int dt = -\frac{D_c \phi}{D_c CA_0} \int \frac{R}{R_o} \frac{dR}{R^2} - \frac{R^2}{R_o}$$

$$\Rightarrow t = -\frac{D_c \phi}{D_c CA_0} \left[\frac{R_o^2}{2} - \frac{1}{R_o} \right]$$

$$\Rightarrow t = -\frac{D_c \phi}{D_c CA_0} \left[\frac{R_o^2}{2} - \frac{R_o^2}{3} \right]$$

$$e = \frac{R_o^2}{6} \frac{P_c \phi}{D_c CA_0}$$

$$t = -\frac{P_c \phi}{D_c CA_0}$$

$$\text{Time taken} = \frac{R_o^2}{D_c CA_0}$$

$$+ = D_c \phi \frac{4\pi R^2}{3}$$

$$c = \frac{R_0^2}{6} \frac{P_c \phi}{D_C C_{AO}}$$

~~$\frac{R_0 - R}{D_C C_{AO}}$~~

$$t = - \frac{P_c \phi}{D_C C_{AO}} \left[\frac{R^2}{2} - \frac{R^3}{3R_0} \right]$$

$$+ \frac{R_0^2 P_c \phi}{6 D_C C_{AO}}$$

$$\text{or } t = \frac{P_c \phi}{D_C C_{AO}} \left[\frac{-R^2}{2} + \frac{R^3}{3R_0} + \frac{R_0^2}{6} \right]$$

Time taken for complete regeneration

$$= \frac{R_0 \rightarrow 0}{\frac{R_0^2 P_c \phi}{6 D_C C_{AO}}} = \frac{R_0^2 P_c \phi}{6 D_C C_{AO}}$$

$$+ = \frac{\phi P_c \phi R_0^2}{6 D_C C_{AO}} \left[1 - 3 \left(\frac{R}{R_0} \right)^2 + 2 \left(\frac{R}{R_0} \right)^3 \right]$$

Oxygen diffuses from R_0 to gas - solid interface

