

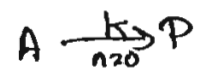
$$\frac{N_A}{V} = \frac{N_{A0}(1-X_A)}{V}$$

for const. vol. Rxn System, $V=V_0$.

$$C_A = \frac{N_{A0}(1-X_A)}{V_0} = C_{A0}(1-X_A)$$

Kinetic Equation for different order of rxn :-

→ for zero order rxn,



$$-r_A = -\frac{dC_A}{dt} = kC_A^{n=0} = k =$$

$$\int_{C_{A0}}^{C_A} -dC_A = \int_0^t k dt$$

$$C_{A0} - C_A = kt$$

$$C_A = C_{A0}(1-X_A)$$

$$C_{A0} X_A = kt$$

$$X_A = \frac{k}{C_{A0}} \cdot t$$

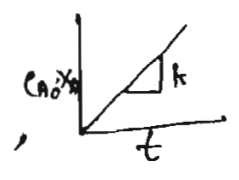
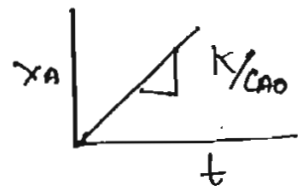
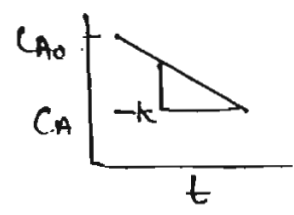
$$\frac{\partial X_A}{\partial t} = \frac{k}{C_{A0}}$$

Conversion depends over initial concentration

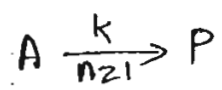
$$C_A = C_{A0} - kt$$

$$y = c + mx$$

$$y = mx$$



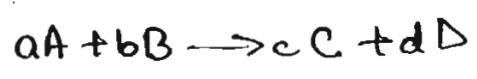
→ for first order rxn,



$$-r_A = -\frac{dC_A}{dt} = kC_A$$

$$k = 1.07 \text{ hr}^{-1}$$

Mole Balance



$$\text{Moles of B reacted} = \frac{\text{Moles of B reacted}}{\text{Moles of A reacted}} \times \text{Moles of A reacted}$$

$$\text{Moles of B reacted} = \frac{b}{a} \times \text{Moles of A Reacted}$$

$$\text{Moles of B unconverted (remaining)} = \text{Moles of B initially fed} - \text{Moles of B reacted}$$

$$N_B = N_{B0} - \frac{b}{a} \text{ Moles of A reacted}$$

$$N_B = N_{B0} - \frac{b}{a} N_{A0} \cdot X_A$$

$$\text{Moles of C In outlet} = \text{Moles of C initially} + \left\{ \frac{c}{a} N_{A0} \cdot X_A \right\} \text{ Moles of C formed}$$

$$N_C = N_{C0} + \frac{c}{a} N_{A0} \cdot X_A$$

$$N_D = N_{D0} + \frac{d}{a} N_{A0} \cdot X_A$$

$$N_A = N_{A0} - N_{A0} \cdot X_A$$

$$\frac{N_A}{V} = \frac{N_{A0} - N_{A0} \cdot X_A}{V}$$

$$\frac{N_B}{V} = \frac{N_{B0} - \frac{b}{a} N_{A0} \cdot X_A}{V}$$

$$N_C = N_{C0} + \frac{c}{a} N_{A0} \cdot X_A$$

$$\int_{C_{A0}}^{-\frac{dC_A}{C_A^2}} = \int_0^t k dt$$

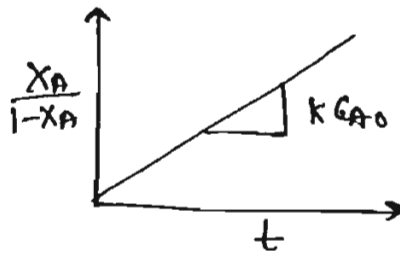
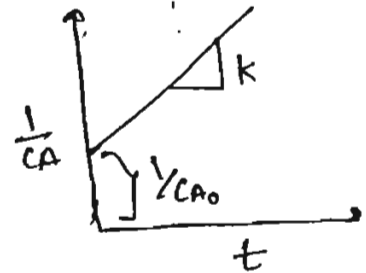
$$\frac{1}{C_A} - \frac{1}{C_{A0}} = kt$$

in terms of conversion.

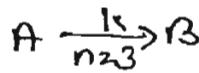
$$C_A = C_{A0}(1 - X_A)$$

$$\frac{X_A}{1 - X_A} = C_{A0} kt$$

$$X_A = \frac{C_{A0} kt}{1 + C_{A0} kt}$$



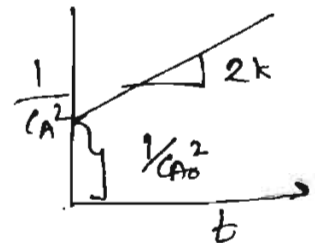
For third order rxn :-



$$-r_A = -\frac{dC_A}{dt} = kC_A^3$$

$$\int_{C_{A0}}^{C_A} -\frac{dC_A}{C_A^3} = \int_0^t k dt$$

$$\frac{1}{C_A^2} - \frac{1}{C_{A0}^2} = 2kt$$



for $n=2 \Rightarrow \frac{1}{C_A} - \frac{1}{C_{A0}} = kt$

for $n=3 \Rightarrow \frac{1}{C_A^2} - \frac{1}{C_{A0}^2} = 2kt$

for n^{th} order rxn, $\frac{1}{C_A^{n-1}} - \frac{1}{C_{A0}^{n-1}} = (n-1)kt$

for all order of rxns this eqn is

for constant vol. system.

$$V = V_0 \\ dV = 0$$

$$r_i = \frac{1}{V} \left[V \cdot \frac{dc_i}{dt} \right]$$

$$r_i = \frac{dc_i}{dt}$$

for reactant A

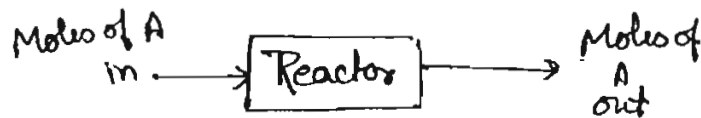
$$r_A = -\frac{dc_A}{dt}$$

for prod P

$$r_P = \frac{dc_P}{dt}$$

Conversion (X) :-

$$X_A = \frac{\text{Moles of A reacted}}{\text{Initial moles of A fed to the system.}}$$



M.B of A

$$\text{Moles of A in} = \text{Moles of A out} + \text{Moles of A reacted.}$$

$$N_{A0} = N_A + \text{Moles of A reacted.}$$

$$\text{Moles of A reacted} = N_{A0} - N_A$$

$$** \quad X_A = \frac{N_{A0} - N_A}{N_{A0}}$$

$$** \quad N_A = N_{A0}(1 - X_A)$$

Valid for both constant & variable volume systems.

$$\int_{C_{A0}}^{C_A} \frac{-dC_A}{C_A} = \int_0^t k dt$$

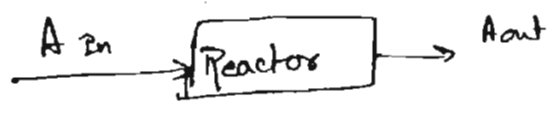
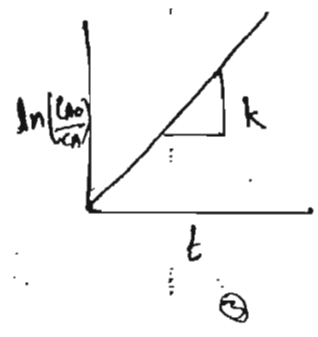
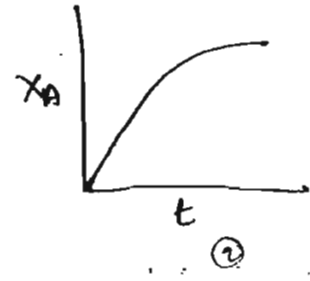
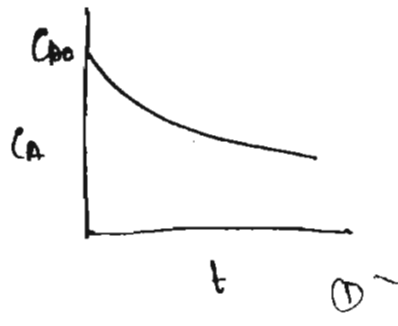
$$\ln(C_{A0}/C_A) = kt$$

$$\textcircled{2} \ln \left(\frac{C_{A0}}{C_A} \right) = kt$$

$$\frac{C_{A0}}{C_A} = e^{kt}$$

$$\textcircled{1} C_A = C_{A0} e^{-kt}$$

$$\textcircled{2} X_A = 1 - e^{-kt}$$

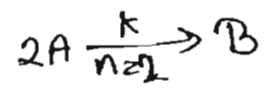


$$X_A = 1 - e^{-kt}$$

$$\frac{\partial X_A}{\partial t} = (-k) e^{-kt}$$

Conversion is independent of initial concentration.

For unimolecular second order rxn:-



$$-r_A = -\frac{dA}{dt} = kC_A^2$$

$$-r_A = \frac{-dC_A}{dt} = kC_A^n$$

$$\int_{C_{A0}}^{C_A} \frac{-dC_A}{C_A^n} = \int_0^t k dt$$

$$-\left\{ \frac{1}{(1-n)C_A^{n-1}} \right\}_{C_{A0}}^{C_A} = kt$$

$$\boxed{\frac{1}{C_A^{n-1}} - \frac{1}{C_{A0}^{n-1}} = (n-1)kt}$$

Q) For the rxn, $A \rightarrow P$. The rate constant is $k = 3.5 \text{ mol/l}\cdot\text{sec}$. Find out the conv. after 15 sec, if C_{A0} was 10 mol/l .

$$C_{A0} X_A = kt$$

$$X_A = \frac{3.5 \times 15}{10} \frac{\text{mol}}{\text{l}\cdot\text{sec}} \cdot \frac{\text{sec}}{\text{mol}}$$
$$= 5.25 \text{ } \cancel{\text{mol}} \cancel{\text{sec}}$$

after 15 sec $X_A = 100\%$

Value greater than 1 but it represent that our rxn has been completed.

time at which rxn was complete

$$1 = \frac{3.5 \times t}{10}$$

$$t = 2.857 \text{ sec}$$

Q) for the liquid phase first order rxn, the conv. was 30% at the end of 20 min and 60% at the end of 35 mins... what will be the initial concn of A and rate const A in (hr^{-1})

$$X_A = 1 - e^{-kt}$$
$$0.30 = 1 - e^{-k \cdot \frac{20}{60}}$$
$$e^{-k \cdot \frac{1}{3}} = 0.7$$

plz
= 1

$$\frac{ND}{V} = \frac{ND_0 + \frac{d_A}{a} NA_0 \cdot X_A}{V}$$

for constant $V = V_0$

$$C_A = \frac{NA_0 - NA_0 \cdot X_A}{V}$$

$$\Rightarrow C_A = C_{A0} - C_{A0} \cdot X_A$$

$$C_B = \frac{NB_0 - \frac{b}{a} NA_0 \cdot X_A}{V}$$

$$\Rightarrow C_B = C_{B0} - \frac{b}{a} C_{A0} \cdot X_A$$

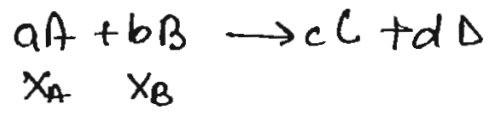
$$C_C = \frac{NC_0 + \frac{c}{a} NA_0 \cdot X_A}{V}$$

$$\Rightarrow C_C = C_{C0} + \frac{c}{a} C_{A0} \cdot X_A$$

$$C_D = \frac{ND_0 + \frac{d}{a} NA_0 \cdot X_A}{V}$$

$$\Rightarrow C_D = C_{D0} + \frac{d}{a} C_{A0} \cdot X_A$$

Constant Volume Rxn System:-



Moles of B reacted = $\frac{b}{a}$ moles of A reacted

$$NB_0 \cdot X_B = \frac{b}{a} NA_0 \cdot X_A$$

$$\frac{NA_0 \cdot X_A}{a} = \frac{NB_0 \cdot X_B}{b}$$

Q. For the rxn $2A + 3B \rightarrow 5C$,

$C_{A0} = 100$, final conc $C_C = 45$.
 $C_{B0} = 100$,
 $C_{C0} = 0$

$X_A, C_A, C_B, X_B = ?$

$$45 = C_{C0} + \frac{5}{2} \times 100 X_A$$

$$45 = C_{C0} + 250 X_A$$

$$C_A = 100 - \frac{3}{2} \times 100 X_A = 100 - 150 X_A$$

$$45 = 0 + 250 X_A$$

$$X_A = 20.18$$

$$C_B = 100 - 150 X_A$$

$$C_B = 73$$

$$C_A = 100(1 - X_A)$$

$$= 82$$

$$X_B = \frac{N_{A0} X_A \cdot a}{N_{B0}} \cdot \frac{b}{a}$$

$$= \frac{C_{A0} \cdot X_A \cdot b}{C_{B0}}$$

for const vol system.

$$= 0.27$$

1666 cm³ min
1 min = 1/60 hr

Sept 7, 14

Q) For a certain rxn, rate exp is given as $-r_A = 0.005 C_A^2 \frac{\text{mol}}{\text{cm}^3 \text{min}}$.
If concn is to be expressed in mol/l & time in hrs, then what will be the units & value of rate constant.

(time)⁻¹ (conc)⁻ⁿ

$$-r_A = 0.005 C_A^2 \text{ mol/cm}^3 \text{ min.}$$

$$\text{min}^{-1} \left(\frac{\text{mol}}{\text{cm}^3} \right)^{-2}$$

$$= 0.005 \frac{\text{mol}}{\text{cm}^3 \text{ min}} \times \frac{1 \text{ cm}^3}{10^6 \text{ ltr}} \times \frac{1 \text{ ltr}}{11} \times \frac{60 \text{ min}}{1 \text{ hr}}$$

$$= 0.005 \frac{\text{cm}^3}{\text{mol} \cdot \text{min}}$$

$$= 0.005 \frac{\text{cm}^3}{\text{mol} \cdot \text{min}} \times \frac{10^6 \text{ ltr}}{1 \text{ m}^3} \times \frac{11}{10^3 \text{ cm}^3} \times \frac{1 \text{ hr}}{60 \text{ min}}$$

$$= 63 \times 10^{-4} \frac{\text{l}}{\text{mol} \cdot \text{hr}}$$

Rxn Mixture

Constant Volume Rxn Systems

The vol of rxn mixture does not change with the rxn progression
(Constant density System)
(liq phase)

Variable Volume Rxn Systems

The vol of the rxn mixture is changed with the rxn progression.
(Variable density System)
(gas rxn)

Constant Volume Systems: -

Concentration: - (c)
moles of solute / volume of solution.

for A,

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

$$N_A = C_A \cdot V$$

$$** \frac{dN_i}{dt} = \frac{1}{V} \frac{dN_i}{dt}$$

$$N_i = C_i V$$

$$\frac{dN_i}{dt} = \frac{1}{V} \frac{d(C_i \cdot V)}{dt}$$

$$= \frac{1}{V} \left(V \frac{dC_i}{dt} + C_i \frac{dV}{dt} \right)$$

general form of rate eqn

for constant volume system.

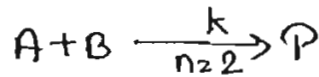
Initial concentration

$$C_{A0} = \frac{N_{A0}}{V_0}$$

Final concentration

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

Kinetic Equation for Bimolecular second order rxn :-



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

$$C_A = C_{A0}(1 - X_A)$$

$$C_B = C_{B0} - \frac{b}{a} C_{A0} X_A$$

$$-\frac{d}{dt} [C_{A0}(1 - X_A)] = k C_{A0}(1 - X_A) (C_{B0} - \frac{b}{a} C_{A0} X_A)$$

$$\Rightarrow C_{A0} \cdot \frac{dX_A}{dt} = k C_{A0}(1 - X_A) (C_{B0} - \frac{b}{a} C_{A0} X_A)$$

$$\Rightarrow \frac{dX_A}{dt} = k(1 - X_A) (C_{B0} - \frac{b}{a} C_{A0} X_A)$$

$$= k(1 - X_A) C_{A0} (\frac{C_{B0}}{C_{A0}} - \frac{b}{a} X_A) \quad \because \frac{b}{a} = \frac{1}{1} = 1$$

$$\boxed{\frac{dX_A}{dt} = k C_{A0}(1 - X_A)(M - X_A)}$$

$$M = \frac{C_{B0}}{C_{A0}}$$

$$\int_0^{X_A} \frac{dX_A}{(1 - X_A)(M - X_A)} = \int_0^t k C_{A0} dt$$

Partial fraction

$$\frac{A + B}{(1 - X_A)(M - X_A)}$$

$$\int_0^{X_A} \left[\frac{1}{(M-1)(1-X_A)} - \frac{1}{(M-1)(M-X_A)} \right] dX_A = \int_0^t k C_{A0} dt$$

$$A(M - X_A) + B(1 - X_A) = 1$$

$$MA + B = 1$$

$$-A - B = 0$$

$$-A = B$$

$$(M-1)A = 1$$

$$A = \frac{1}{(M-1)}$$

$$B = -\frac{1}{(M-1)}$$

$$\frac{1}{(M-1)} \left\{ \int_0^{X_A} \frac{dX_A}{(1-X_A)} - \int_0^{X_A} \frac{dX_A}{(M-X_A)} \right\} = k C_{A0} t$$

$$\frac{1}{(M-1)} \left\{ -\ln(1-X_A) \Big|_0^{X_A} - \left[-\ln(M-X_A) \Big|_0^{X_A} \right] \right\} = k C_{A0} t$$

$$- \left[\ln(1-X_A) - \ln(1-0) \right] + \left[\ln(M-X_A) - \ln(M-0) \right] = (M-1) k C_{A0} t$$