Reaction - Diffusion Systems

(IMSE → Belgia) (International micro-)

Silican can have 2-3% impurities.

$10^{19} - 10^{20}$ (1 atom impure)

- In nanotechnalogy, purity is defined as atom.

- FAB / silican chip
- lithography & photografhy.

$$xA + yB \rightarrow aC + bD.$$

① rate of reaction $\propto [A]^{\alpha}[B]^{\beta}$.

② $$\frac{(-r_A)}{x} = \frac{(-r_B)}{y} = \frac{(+r_C)}{a} = \frac{(+r_D)}{b}$$

③ $$-\frac{1}{x}\frac{dC_A}{dt} = -\frac{1}{y}\frac{dC_B}{dt} = \frac{1}{a}\frac{dC_C}{dt} = \frac{1}{b}\frac{dC_D}{dt}.$$

- Dividing with moles to equal the rate of reaction of each agents participating in the reaction.

Arrhenius Theory →

$$K = Ae^{-E/RT}.$$

- Collision, molecularity ≤ 3, elementary rxn.

A + B → Products

Monday

$A + B \rightarrow$ Products

Data

Exp	Conc. A (M)	Conc. B (M)	Initial rate (s^{-1})
1	0.1	0.2	9×10^{-4}
2	0.1	0.4	1.8×10^{-3}
3	0.05	0.2	2.25×10^{-4}

for first order rxn :-

$$\cancel{(-r_A) = KC_A}$$
$$\cancel{(-r_B) = KC_B}$$

$$\cancel{(-r_A) \neq (-r_B)}$$

rate $(-r) = KC_A^{\alpha} C_B^{\beta}$

$$(-r_1) = 9 \times 10^{-4} = K (0.1)^{\alpha} (0.2)^{\beta} \quad -(1)$$
$$(-r_2) = 1.8 \times 10^{-3} = K (0.1)^{\alpha} (0.4)^{\beta} \quad -(2)$$

(1)/(2) ;

$$\left(\frac{0.2}{0.4}\right)^{\beta} = \frac{90}{18} \times 10^{-1} = \frac{9}{18}$$

$$\left(\frac{1}{2}\right)^{\beta} = \left(\frac{1}{2}\right)$$

$$\boxed{\beta = 1}$$

Similarly;

$$(r_1) = 9 \times 10^{-4} = K (0.1)^{\alpha} (0.2)^{\beta} \quad -(3)$$
$$(r_3) = 2.25 \times 10^{-4} = K (0.05)^{\alpha} (0.2)^{\beta} \quad -(4)$$

8) (4) ;

$$\left(\frac{9}{2.25}\right) = \left(\frac{0.1}{0.05}\right)^{\alpha}$$

$$\left(\frac{900}{225}\right) = \left(\frac{\cancel{10}^{2}}{5}\right)^{\alpha}$$

$$2^{\alpha} = 2^{2}$$

$$\boxed{\alpha = 2}$$

rate expression;

$$(-r) = K C_A^{\alpha} C_B^{\beta}$$

$$(-r) = K C_A^{2} C_B^{1}$$

$$\cancel{\frac{r_1}{r_2} = 9\times10^{-4}}$$

$$\because \quad r_1 = 9\times10^{-4} = k(0.1)^2(0.2)^1$$

$$K = \frac{9\times10^{-4}}{10^{-2}\times0.2} = \frac{9}{0.2}\times10^{-2} = \frac{90}{2}\times10^{-2}$$

$$K = 45\times10^{-2} = 0.45$$ //

Rate expression →

$$\text{rate} = 0.45\, C_A^{2} C_B^{1}$$ //

$H_2 + Br_2 \longrightarrow 2HBr$

$Br_2 \xrightarrow{k_1} Br^*$

$Br^* + H_2 \longrightarrow HBr^* + H^*$

~~$H^* + Br^* \longrightarrow HBr$~~

<u>Method</u> → steady state approximation.

$Br_2 \xrightarrow{k_1} Br^*$

$Br^* + H_2 \xrightarrow{k_2} HBr + H^*$

$H_2 + Br^* \xrightarrow{k_4} HBr + H^*$

$H^* + Br_2 \xrightarrow{k_3} HBr + Br^*$

$2Br^* \xrightarrow{k_1} Br_2$

$H_2 + Br^* + \cancel{H^*} + Br_2 + \cancel{Br} \longrightarrow 2HBr + \cancel{H^*} + \cancel{Br} + \cancel{Br_2}$

$r_{HBr} = k_2 . [Br]^* [H_2]$

$r_{Br^*} = k_1 [Br_2] - k_2 [Br^*]$

At equilibrium, $r_{Br^*} = 0$.

$[Br^*] = \frac{k_1}{k_2} [Br_2]$.

$r_{HBr} = k_2 . \frac{k_1}{k_2} [Br_2][H_2]$

$$Br_2 \xrightarrow{k_1} Br^*.$$

$$Br^* + H_2 \xrightarrow{k_2} \cancel{HBr + H^*}.$$

$$H^* + HBr \xrightarrow{k_4} H_2 + Br^* \quad -(1)$$

$$H^* + Br_2 \xrightarrow{k_3} HBr + Br^* \quad -(2)$$

$$2Br^* \xrightarrow{k_1} Br_2. \quad -(3):$$

$$r_{HBr} = k_4 [H^*][HBr] + k_3 [H^*][Br_2]$$

$$\cancel{r_{Br^*} = k_4 [Br^*]^2}.$$

$$r_{Br^*} = k_4 [H^*][HBr] - k_1 [Br^*]^2 + k_3 [H^*][Br_2]$$

$$r_{Br_2} = k_1 [Br^*]^2 - k_3 [H^*][Br_2].$$

<u>At s.s →</u>

$$r_{Br_2} = 0$$

$$k_1 [Br^*]^2 = k_3 [H^*][Br_2].$$

$$\therefore r_{Br^*} = 0.$$

$$\Rightarrow k_4 [H^*][HBr] + k$$

$2H^* + 2HBr + \cancel{2Br^*} \rightarrow H_2 + \cancel{2Br^*} + \cancel{HBr} + Br_2$

$+Br_2$

$\cancel{2HBr} \rightarrow$

$\cancel{H_2}$

$$Br_2 \xrightarrow{k_1} 2Br^*$$

$$Br^* + H_2 \xrightarrow{k_2} HBr + H^*$$

$$H^* + HBr \xrightarrow{k_4} H_2 + Br^*$$

$$H^* + Br_2 \xrightarrow{k_3} HBr + Br^*$$

$$\cancel{2Br^* \xrightarrow{k_5} Br_2}$$

$$\cancel{Br_2} + \cancel{H_2} + \cancel{Br^*} + \cancel{H^*} + \cancel{HBr} + H^* + Br_2 + \cancel{2Br^*}$$
$$\rightarrow \cancel{2Br^*} + HBr + \cancel{H^*} + \cancel{H_2} + \cancel{Br^*} + \cancel{HBr} + Br^* + \cancel{Br_2}$$

$$\cancel{H^* + Br_2 \rightarrow HBr + Br^*}$$

$$r_{HBr} = k_2[Br^*][H_2] - k_4[H^*][HBr] + k_3[H^*][Br_2]$$

$$r_{Br^*} = k_1[Br_2] - k_2[Br^*][H_2] + k_4[H^*][HBr] + k_3[H^*][Br_2]$$

$$r_{H^*} = k_2[Br^*][H_2] - k_4[H^*][HBr] - k_3[H^*][Br_2]$$

$$r_{H^*} = 0 \qquad k_4[H^*][HBr] = k_2[Br^*][H_2] - k_3[H^*][Br_2] \qquad (1)$$

$\cancel{[Br^*] =}$

$$r_{HBr} = k_2[Br^*][H_2] - k_2[Br^*][H_2] + 2k_3[H^*][Br_2]$$

$$\boxed{r_{HBr} = 2k_3[H^*][Br_2]}$$

$$r_{Br^*} = 0.$$

$$k_1[Br_2] - k_2[Br^*][H_2] + k_4[H^*][HBr] = -k_3[H^*][Br_2].$$

k_1

$$k_3[H^*][Br_2] = k_3[H^*][Br_2] - k_1[Br_2].$$

$$k_1[Br_2] = 0.$$

$$\Rightarrow \quad k_4[H^*][HBr] + k_3[H^*][Br_2] = k_2[Br^*][H_2]$$

$$[H^*]\left[k_3[Br_2] + k_4[HBr]\right] = k_2[Br^*][H_2]$$

$$[H^*] = \frac{k_2[Br^*][H_2]}{k_3[Br_2] + k_4[HBr]} \quad (1)$$

$$r_{HBr} = k_2[Br^*][H_2] + [H^*]\left[k_3[Br_2] - k_4[HBr]\right]$$

$$r_{HBr} = k_2[Br^*][H_2] + \frac{k_2[Br^*][H_2]\left[k_3[Br_2] - k_4[HBr]\right]}{k_3[Br_2] + k_4[HBr]}.$$

$$r_{HBr} = \left(k_4[HBr] + k_3[Br_2]\right)\left\{1 + \frac{k_3[Br_2] - k_4[HBr]}{k_3[Br_2] + k_4[HBr]}\right\} ?$$

$K_2 \cancel{[Br^*][H_2]} =$

$$\begin{cases} r_{HBr} = k_2[Br^*][H_2] + K_3[H^*][Br_2] \\ r_{H^*} = k_2[Br^*][H_2] \\ r_{Br^*} = K_4[H^*][HBr] + K_3[H^*][Br_2] + K_1[Br_2] \end{cases}$$

$$K_3[H^*][Br_2] = -K_1[Br_2].$$

Sequential rxn

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C. \qquad ((k_2 >>> k_1), (+r_B) = 0.)$$

$$[C] = [A_0][\quad]$$

$$C_c = C_{B_0} + C_{A_0} \cdot X_A \quad ;$$

$$C_c = C_{A_0}(1 + X_A)$$

$$[C] = [C]_0 + [A]_0 \cdot X_A. \qquad ([A]_0 = [C]_0)$$

$$\left\{ X_A = 1 - \frac{[A]}{[A_0]} \right\}$$

$$\boxed{[C] = [A]_0[1 + X_A]}$$

$$[C] = [A]_0\left[2 - \frac{[A]}{[A]_0}\right]$$

$\cancel{[C] = [A]_0[2 - e^{-k_1 t}]}$

$(-r_A) = k_1 [A].$

$(+r_B) = k_1 [A].$

$(+r_C) = k_2 [B].$

$[B] = [B]_0 + [A]_0 \cdot X_A.$

$\Rightarrow \quad k_1 [A] = \frac{d[A]}{dt}$

$$\Rightarrow \quad \int_{A_0}^{A} \frac{d[A]}{[A]} = \int k_1 dt$$

$$\{\ln [A] - \ln [A_0]\} = k_1 t + C.$$

$$\ln \frac{[A]}{[A]_0} = k_1 t.$$

$$\{ [A] = [A]_0 e^{k_1 t} \} - ①.$$

$$[C] = [A]_0 \left[2 - \frac{[A]_0 e^{k_1 t}}{[A]_0} \right]$$

$$\boxed{[C] = [A]_0 \left[2 - e^{k_1 t} \right]} - ②$$

$\Rightarrow \quad \cancel{\frac{d[C]}{dt}}$

$\{ [B] = [B]_0 + [A]_0 X_A \}$

$\Rightarrow \quad \frac{d[B]}{dt} = k_1 [A]$

$\Rightarrow \quad \cancel{d\{[B]_0 + [A]_0 X_A\} = k_1 [A]_0 (1 - X_A)\, dt.}$

$\Rightarrow \quad \cancel{\frac{dX_A}{dt} = k_1 (1 - X_A)}$

$\cancel{-\ln(1 - X_A) = k_1 t}$

$e^{-k_1 t} = \frac{[A]}{[A_0]}$

$$\frac{d[C]}{dt} = k_2[B]$$

$$[B] = [B]_0 + [A]_0 x_A$$

$$\frac{d[C]}{dt} = k_2\{[B]_0 + [A]_0 x_A\}$$

$$d[C] = k_2[B]_0 + k_2[A]_0 x_A \, dt$$

$$r_B = k_1[A]$$

$$\frac{d[B]}{dt} = k_1[A]$$

$$\frac{d\{[B]_0 + [A]_0 x_A\}}{dt} = k_1[A]$$

$$[A]_0 \frac{dx_A}{dt} = k_1$$

Diffusian

→ For the case of rxn diffusian system.

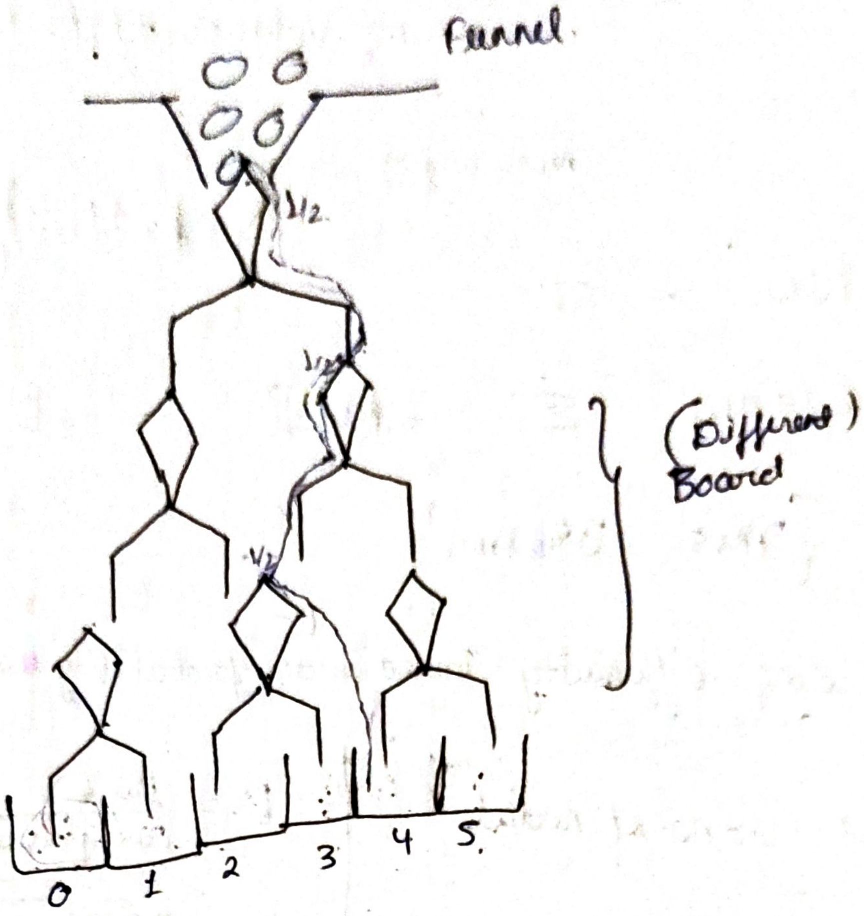
→ Browmian motion. (Randomness of particles).

↳ (19th century, Robert Brown)

↳ small particle random motion in the water in beaker.

↳ Random walk / Diffusion model → (Applicable to all random motion in space)

e.g. Galton Board.



$x \to 1/2$

$n \to$ no of terms.

$\left(\frac{n}{2} \times \frac{1}{x}\right) \Rightarrow \frac{n}{2} + \frac{n}{2} =$

$\Rightarrow$

$\Rightarrow \quad = \frac{A}{2} \times$

$\Rightarrow \quad = \frac{1}{\frac{n}{2} \times 1/2} = \frac{1}{2} \quad \frac{2}{nx}$

$= \frac{2}{48 \times 4} = \frac{1}{16}$

$\Rightarrow 8 - 3$

$\Rightarrow n \; (n-5) \times \frac{1}{2} + \frac{x}{2}$

$\frac{3}{2} + \frac{6}{2} = \frac{9}{2}$

$\Rightarrow$

$p \rightarrow$ probability of a particle from origin moving distance $\pm l$. particle travels

Mean avg $\Rightarrow$ $\{ \cdot p, \pm l, \delta \}$

Mean $=$

Variance: $\Sigma \quad - \text{Mean})^2$

$\{ rms = \delta \, x_{rms} \}$

→ Finding diffusivity based on the probability value →

→ n = no. of Particle

→ Mean, Variance, rms.

$D = \dfrac{\text{flux}}{\text{conc. gradient}}$

$N_A = D \dfrac{\partial C_A}{\partial x}$

rms = root mean square $=$

$= \sqrt{\Sigma \delta^2}$

$\tau \Rightarrow$ one time step

$t \Rightarrow$ Total time.

$= \sqrt{\Sigma x_i^2}$

Mean $= pl(1-pl)$

$\Rightarrow$ Mean $= pl(1-p)$

Variance $= \sigma^2 = \Sigma pl^2 - (pl(1-pl))^2$

Mean avg value for n particles $= pl_i(1-p)$

$\bar{\mu} = pl(1-pl)$

τ → time step.

t → Total time.

n → no. of particles

$\overset{\tau}{0 \longrightarrow t}$ → m^2/sec.

Distance covered in t time

Dis = speed x time

Distance $= \left(\frac{l}{\tau}\right) \times t) \times n$.

n → no. of particles.

$$D = \frac{(nl) \times t \times nl/\tau}{}$$

$$D = \frac{n^2 l^2}{\tau}$$

Assumption → all particles ~~travels~~ equal distance in 'l'

τ time. $(nl) \times n$.

→ same speed → (l/τ) ? {change in length

$$D = \frac{\text{flux}}{\partial C / \partial x} = \frac{(nl)}{\partial C / \partial x}$$

Assumption

. Each particle have independent time step.

$D = m^2/sec$ → (Each particle cover distance in single time step) x (Total distance cover)

D =

Mean for n particles → $pl(1-pl)$
(1st particle)

1 particle → mean
1 particle → τ_1
τ_1 → mean
$\left(1 \to \frac{mean}{\tau}\right)$

For n-particles → $\sum_{i=1}^{n} \frac{p_i l(1-p_i l)}{\tau_i}$

Variance for n-particles → $\sum_{i=1}^{n} \frac{p_i^2 l^2 (1-p_i l)^2}{\tau_i^2} - (mean)^2$

~~Diffusivity~~ → ~~For Variance~~ simple

$D = \cancel{\sum \frac{p_i l^2 (1-p_i l)^2}{\tau_i}}$

m^2/sec

Mean of n-particles for total time t → $\frac{\sum_{i=1}^{n} p_i l(1-p_i l)}{\sum_{i=1}^{n} \tau_i}$

Diffusivity $= \frac{\sum_{i=1}^{n} p_i l(1-p_i l)}{n\tau_i}$ $\quad t = \frac{\sum_{i=1}^{n} p_i l}{n\tau}$

Total time $= \frac{n l}{n\tau} \Rightarrow \frac{n p_i l}{n\tau}$

$t = \frac{p_i l}{\tau}$ $\quad \tau = \frac{t}{p_i l}$

m^2/sec

$= p_i l(1-p_i l)$

$n\tau = \frac{t}{\sum_{i=1}^{n} p_i l}$

$$D = \frac{\sum_{i=1}^{n} p_{id}(1-p_{id})}{t} \quad \left(\Sigma p_{id}\right)$$

$t \rightarrow n\tau$

$t \propto \tau$

$$\boxed{1 \rightarrow \frac{n\tau}{t}}$$

$$\sum_{i}^{m} p_{id}(1-p_{id}) \times \frac{n\tau}{t}$$

τ time step.

Total time → $n\tau$ time step)

$t \rightarrow n\tau$

$$D = \sum_{i=1}^{n} p_{id}(1-p_{id}) \times \frac{n\tau}{t^2} \qquad \left(1 \rightarrow \frac{n\tau}{t}\right)$$

$$D = \sum_{i=1}^{n} p_{id}(1-p_{id}) \times \frac{n\tau}{t}$$

Mean: $\mu = \sum_{i=1}^{n} l \cdot p_i$

Variance: $\sigma^2 = \sum_{i=1}^{n} l^2 p_i - \mu^2$

Solutions

Given → • The particle undergoes a biased random walk.

• The distance per step is

$$\Delta = \begin{cases} l, & \text{with probability } p \\ -l, & \text{with probability } 1-p. \end{cases}$$

• Particle starts from origin

• Particle moves a distance l during time interval τ.

(i) Mean distance

$$\bar{\mu} = \sum_{i=1}^{n} E|\Delta_i|$$

$$\bar{\mu} = \sum_{i=1}^{n} [l p_i + (-l)(1-p_i)]$$

$$\bar{\mu} = \sum_{i=1}^{n} [l p_i - l + l p_i]$$

$$\bar{\mu} = \sum_{i=1}^{n} [l(1-2p_i)] \;//$$

Since all steps are independent, the mean for n-particles step is.

$$\bar{\mu} = nl(1-2p)$$

where, $n = t/\tau$

$$\boxed{\bar{\mu} = \frac{tl(1-2p)}{\tau}} - (1)$$

(ii) Variance of Distance

$$\sigma^2 = E[l_i(n)^2] - [E(l_i(n))]^2$$

$$\cancel{\sigma^2 = nl^2 + n(n-1)l^2}$$

$$E[l_i(n)^2] = l^2[1-p+p] = l^2$$

Summing over n-steps.

$$\sum_{i=1}^{n} E[l_i(n)]^2 = nl^2$$

$$E[l_i(n)^2] = \sum_{i=1}^{n} E[l_i^2] + 2\sum_{i<j} E(l_i l_j)$$

Since the steps are independent

$$E(l_i l_j) = E(l_i)\,E(l_j) = \sum_{i<j} l^2/9.$$

Using summation formula →

$$\sum_{i<j} 1 = \frac{n(n-1)}{2}$$

$$\sum_{i<j} \frac{l^2}{9} = \frac{n(n-1)}{2} \cdot \frac{l^2}{9} = \frac{n(n-1)l^2}{18}$$

$$E(l_i(n)^2) = nl^2 + \frac{n^2 l^2}{9} = \frac{1}{c} l^2$$

For n-particle →

$$\sigma^2 = nl^2 + \frac{n(n-1)l^2}{9} - \left(\frac{nl}{9}(1-p)\right)^2$$

$$\sigma^2 = nl^2 + n(n-1)l^2 p(1-p) - n^2 l^2 (1-p)^2$$

$$\sigma^2 = nl^2 - nl^2 p(1-p)$$

$$\sigma^2 = nl^2(1-p+p^2) \quad -(2)$$

Diffusivity Expression

$$D = \lim_{t \to \infty} \frac{Var[x_i(n)]}{2t}$$

$$D = \lim_{t \to \infty} \frac{t/\tau \, l^2 p(1-p)}{2t}$$

$$\boxed{D = \frac{l^2 p(1-p)}{\tau}}$$

Reaction-Diffusion system →

$$\frac{\partial C_a}{\partial t} = D\left(\frac{\partial^2 C_a}{\partial x^2} + \frac{\partial^2 C_a}{\partial y^2} + \frac{\partial^2 C_a}{\partial z^2}\right)$$

$$\frac{\partial C_a}{\partial t} = \sum_{i=1}^{n} D_{ij} \frac{\partial^2 C_{ai}}{\partial x_j^2} +$$ (Diffusion & Reaction)

$$\frac{\partial C_a}{\partial t} = -\sum_{i=1}^{n} D_{ij}\left(\frac{\partial^2 C_{ai}}{\partial x_j^2} + \frac{\partial^2 C_{ai}}{\partial y_j^2} + \frac{\partial^2 C_{ai}}{\partial z_i^2}\right) + (-r_A).$$

$\frac{m^2}{s} \times \frac{mol}{m^2 \cdot m^3}$

Autocatalytic rxn →

$$\left\{\begin{array}{l} A + B \xrightarrow{k_1} A + B \\ (-r_A) = K_1 C_A C_B \end{array}\right\}$$

$r_A = \frac{-\partial C_a}{\partial t}$ $\left(\frac{mol}{m^3 sec}\right)$

$\frac{mol}{m^3 sec}$ $\frac{mol^3}{m^3 \cdot x}$ $\frac{mol}{m^3}$

Mole Balance:

$$V \frac{\partial C_a}{\partial t} = D \cdot \frac{\partial^2 C_a}{\partial x^2} + (-r_A) \cdot V$$

$(-r_A) = K C_A^{m} C_B^{n}$

$(+r_B) =$

$$\frac{\partial C_A}{\partial t} = -D\frac{\partial^2 C_A}{\partial x^2} + (-r_A)$$

$K C_A^m C_B^n$

$$\frac{\partial C_A}{\partial t} = -D\left(\frac{\partial^2 C_A}{\partial x^2} + \frac{\partial^2 C_A}{\partial y^2} + \frac{\partial^2 C_A}{\partial z^2}\right) + (-r_A)$$

$$\left\{\frac{\partial C_B}{\partial t} = (+r_B) = K C_A^m C_B^n\right\}$$

(0.1)

more less

$(-r_A) = K C_A^m C_B^n \rightarrow$ less.

$$(+r_B) = \frac{\partial C_B}{\partial t} \rightarrow 0.$$

$(-r_A)$

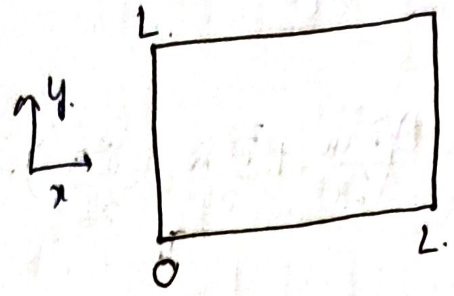
$$\frac{\partial C_A}{\partial t} = -D\left(\frac{\partial^2 C_A}{\partial x^2} + \frac{\partial^2 C_A}{\partial y^2} + \frac{\partial^2 C_A}{\partial z^2}\right) + K C_A^m C_B^n$$

$$\frac{\partial C_B}{\partial t} = -D\left(\frac{\partial^2 C_B}{\partial x^2} + \frac{\partial^2 C_B}{\partial y^2} + \frac{\partial^2 C_B}{\partial z^2}\right) + (+r_B)$$

A → rate of production

B → rate of disappearance.

first order reaction →



$C = f(x, y, t)$

$$\cancel{\frac{\partial c}{\partial t}}^{\,0} = -D\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2}\right) \pm KC$$

B.C's

- $C(0, y, t) = 0$ steady-state
- $C(L, y, t) = 0$
- $C(x, 0, t) = 0$
- $C(x, L, t) = f(x)$

$$\Rightarrow -D\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2}\right) = -KC$$

$$\Rightarrow \left[\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} = \frac{KC}{D}\right] \quad (1)$$

$K/D = (K/D)$

$$\Rightarrow \frac{1}{C}\frac{\partial^2 c}{\partial x^2} + \frac{1}{C}\frac{\partial^2 c}{\partial y^2} = K/D$$

$(D^2 - \lambda^2)C = 0$

$$\Rightarrow \frac{1}{C}\frac{\partial^2 c}{\partial x^2} = K/D - \frac{1}{C}\frac{\partial^2 c}{\partial y^2} = \lambda^2 \text{ (say)}$$

$$\Rightarrow \frac{\partial^2 c}{\partial x^2} - c\lambda^2 = 0$$

$$\Rightarrow \frac{1}{C}\frac{\partial^2 c}{\partial x^2} = \lambda^2$$

$$\Rightarrow [\ln C]\,\frac{\partial c}{\partial x} = \lambda^2 x + C_1$$

Non-dimensionless form eq^n ① →

$$\bar{x} = \frac{x}{L}, \quad \bar{y} = \frac{y}{L}, \quad \bar{c} = \frac{c}{c_m}$$

(Damkohler No → K/D.)

$$\Rightarrow \frac{c_m}{L^2}\frac{\partial^2 \bar{c}}{\partial \bar{x}^2} + \frac{c_m}{L^2}\cdot\frac{\partial^2 \bar{c}}{\partial \bar{y}^2} = K/D.$$

$$\Rightarrow \left[\frac{\partial^2 \bar{c}}{\partial \bar{x}^2} + \frac{\partial^2 \bar{c}}{\partial \bar{y}^2} = \frac{KL^2}{c_m D}\right] \rightarrow ②$$

$\frac{KL^2}{c_m D} \rightarrow K'$

(say)

$$\Rightarrow \left\{\frac{\partial^2 \bar{c}}{\partial \bar{x}^2} + \frac{\partial^2 \bar{c}}{\partial \bar{y}^2} = K'\right\} \qquad \bar{c}(\bar{x},\bar{y}) = X(\bar{x})\cdot Y(\bar{y}).$$

don't su

$$\Rightarrow \frac{\partial^2 \bar{c}}{\partial x^2} = K' - \frac{\partial^2 \bar{c}}{\partial \bar{y}^2} = \lambda^2 \text{ (say)}.$$

$$\Rightarrow \frac{\partial^2 \bar{c}}{\partial x^2} - \lambda^2 = 0$$

$$\Rightarrow \frac{\partial \bar{c}}{\partial \bar{x}} = \lambda\bar{x} + c_1$$

$$\Rightarrow \left\{\bar{c} = \frac{\lambda\bar{x}^2}{2} + c_1\bar{x} + c_2\right\}$$

$$\frac{\partial^2 \bar{c}}{\partial \bar{x}^2} + \lambda^2 \bar{c} = \lambda^2$$

$$\frac{\partial^2 \bar{c}}{\partial \bar{x}^2} + \lambda^2)$$

$$\bar{c} = \bar{x} + \bar{y} + \bar{c}$$

@ $\bar{c}(\bar{x},\bar{y},t) \rightarrow$

@ $\bar{x} = 0,\ \bar{c} = 0$

$\bar{x} = 1,\ \bar{c} = f(\bar{x})$

$\Rightarrow \boxed{c_2 = 0}$

$$\bar{c} = \frac{\lambda\bar{x}^2}{2} + c_1\bar{x}$$

$$f(\bar{x}) = \frac{\lambda}{2} + c_1$$

$$\boxed{c_1 = f(\bar{x}) - \frac{\lambda}{2}}$$

$$\bar{C} = \frac{\lambda \bar{x}^2}{2} + \left(f(\bar{x}) - \frac{\lambda}{2}\right)\bar{x}. \quad -(1)$$

Now, $\quad K' - \frac{\partial^2 \bar{C}}{\partial y^2} = \lambda^2. \qquad (\lambda^2 - K' = \alpha^2)$

$$\frac{\partial^2 \bar{C}}{\partial y^2} + (\lambda^2 - K') = 0.$$

$$\frac{\partial^2 \bar{C}}{\partial y^2} = -\alpha.$$

$$\boxed{\bar{C} = \frac{-\alpha \bar{y}^2}{2} + C_1 \bar{y} + C_2}$$

@ $\bar{y} = 0, \bar{C} = 0.$

$\bar{y} = 1, \bar{C} = 0.$

$$\Rightarrow \quad 0 = 0 + 0 + C_2$$

$$\boxed{C_2 = 0}$$

$$\Rightarrow \quad \bar{C} = -\frac{\alpha \bar{y}^2}{2} + C_1 \bar{y} + 0.$$

$$\Rightarrow \quad 0 = \frac{-\alpha}{2} + C_1$$

$$\boxed{C_1 = \alpha/2}$$

$$\boxed{\bar{C} = \frac{-\alpha \bar{y}^2}{2} + \frac{\alpha}{2}\bar{y}}$$

$$\bar{C}(\bar{x}, \bar{y}) = \left[\frac{\lambda \bar{x}^2}{2} + f(\bar{x})\bar{x} - \frac{\lambda}{2}\bar{x}\right]\left[-\frac{\alpha}{2}\bar{y}^2 + \alpha \bar{y}\right].$$

$$C(x,y) = \left(\frac{\lambda x^2}{L^2 2} + \frac{f(x).x}{L} - \frac{\lambda x}{L.2}\right)\left(\frac{-\alpha y^2}{L^2 2} + \frac{\alpha y}{L}\right)$$

$$C(x,y) = \left[\frac{\lambda x^2}{2L^2} + \frac{x}{L}\left(f(x) - \frac{\lambda}{2}\right)\right]\left[\frac{-\alpha}{2}\left(\frac{y}{L}\right)^2 + \alpha\left(\frac{y}{L}\right)\right]$$

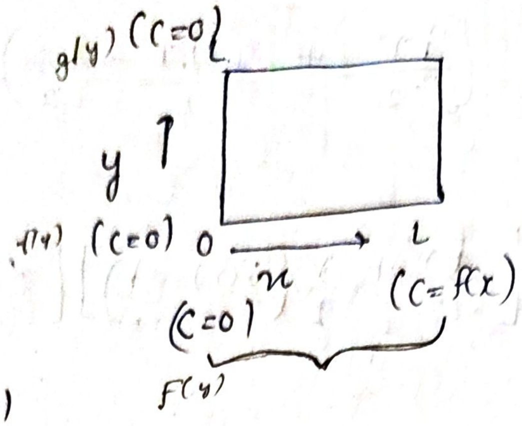
$$C(x,y) = \left[\frac{\lambda}{2}\left(\frac{x}{L}\right)^2 + \left(f(x) - \frac{\lambda}{2}\right)\left(\frac{x}{L}\right)\right]\left[\frac{-\alpha}{2}\left(\frac{y}{L}\right)^2 + \alpha\left(\frac{y}{L}\right)\right]$$

where. $\alpha = \lambda - K'$

$$K' = \frac{KL^2}{DC_m}$$

$$\frac{\partial^2 \bar{C}}{\partial \bar{x}^2} + \frac{\partial^2 \bar{C}}{\partial \bar{y}^2} = A$$

Problem →



$\text{Conc} = f(x, y, t)$

B.C's

$c(0, y, t) = 0$	$c(x, 0, t) = 0$	steady-state
$c(L, y, t) = f(x)$	$c(x, L, t) = 0$	

Eqn:- $\cancel{\dfrac{\partial c}{\partial t}}^{\,0} = D\left(\dfrac{\partial^2 c}{\partial x^2} + \dfrac{\partial^2 c}{\partial y^2}\right) + KC$ {Reaction & diffusion case}

(s-s).

$$\Rightarrow \quad D\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2}\right) + KC = 0 \quad -(1)$$

Non-dimension form → $\left[\bar{x} = \dfrac{x}{L},\ \bar{y} = \dfrac{y}{L},\ \bar{c} = \dfrac{c}{C_m}\right]$

$$\Rightarrow \quad D\left[\frac{C_m}{L^2}\left(\frac{\partial^2 \bar{c}}{\partial \bar{x}^2} + \frac{\partial^2 \bar{c}}{\partial \bar{y}^2}\right)\right] + \bar{c}K\cancel{C_m} = 0$$

$$\Rightarrow \quad \frac{D}{L^2}\left[\frac{\partial^2 \bar{c}}{\partial \bar{x}^2} + \frac{\partial^2 \bar{c}}{\partial \bar{y}^2}\right] + K\bar{c} = 0.$$

$$\Rightarrow \quad \frac{\partial^2 \bar{c}}{\partial \bar{x}^2} + \frac{\partial^2 \bar{c}}{\partial \bar{y}^2} = \frac{-K\bar{c}L^2}{D}.$$

{Damkohler no. $= \dfrac{KL^2}{D}$}

$\left(Da = \dfrac{\text{Mixing time scale}}{\text{Chemical time scale}}\right)$

$$\Rightarrow \quad \frac{\partial^2 \bar{c}}{\partial \bar{x}^2} + \frac{\partial^2 \bar{c}}{\partial \bar{y}^2} = -Da\,\bar{c}$$

$$\Rightarrow \quad \boxed{\frac{\partial^2 \bar{c}}{\partial \bar{x}^2} + \frac{\partial^2 \bar{c}}{\partial \bar{y}^2} + Da\,\bar{c} = 0}$$

Using separation variable Method -

$$\bar{C}(\bar{x},\bar{y}) = X(\bar{x}).Y(\bar{y}) \quad -(2)$$

$$\Rightarrow \quad Y\frac{\partial^2 X}{\partial \bar{x}^2} + X\frac{\partial^2 Y}{\partial \bar{y}^2} + Da\,XY = 0$$

$$\Rightarrow \quad \frac{1}{X}\frac{\partial^2 X}{\partial \bar{x}^2} + \frac{1}{Y}\frac{\partial^2 Y}{\partial \bar{y}^2} + Da = \pm\lambda^2$$

$$\Rightarrow \quad \frac{1}{X}\frac{\partial^2 X}{\partial x^2} = -\lambda^2 = -\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} - Da.$$

$$\Rightarrow \quad \frac{d^2X}{dx^2} + \lambda^2 X = 0$$

$$(D^2+\lambda^2)X = 0$$

$$D = \pm\lambda i$$

$$X(\bar{x}) = C_1\cos(\lambda\bar{x}) + C_2\sin(\lambda\bar{x})$$

@ $\bar{x}=0,\ X=0,\ C_1=0$

$$X(\bar{x}) = C_2\sin(\lambda\bar{x})$$

@ ~~$\bar{x}=1a\ \bar{C}=f(\bar{x})$~~ ~~$C_1\cos(\lambda\bar{x})=0$~~ ~~$\cos(\lambda\bar{x})=$~~ [illegible]

$\bar{x}=1,\ X=0$

$$0 = C_1\overset{\to 0}{\cos(\lambda)} + C_2(\sin\lambda)$$

$$\sin\lambda = 0$$

$$\lambda = n\pi$$

$$\therefore \quad \boxed{X(\bar{x}) = C_2\sin(n\pi\bar{x})} \quad -(3)$$

Now; $$-\frac{1}{Y}\frac{\partial^2 Y}{\partial \bar{y}^2} - Da = -\lambda^2$$

$$\frac{1}{Y}\frac{\partial^2 Y}{\partial \bar{y}^2} + Da = n^2\pi^2$$

$$\frac{1}{Y}\frac{\partial^2 Y}{\partial \bar{y}^2} = n^2\pi^2 - Da.$$

$$\Rightarrow \quad \frac{d^2Y}{d\bar{y}^2} + (Da - n^2\pi^2)Y = 0$$

$$\Rightarrow \quad \frac{d^2Y}{d\bar{y}^2} - (n^2\pi^2 - Da)Y = 0$$

$$\Rightarrow \quad Y(\bar{y}) = C_3 e^{(n^2\pi^2 - Da)^{1/2}\bar{y}} + C_4 e^{-(n^2\pi^2 - Da)^{1/2}\bar{y}}$$

@ $\bar{y}=0,\ Y=0 \Rightarrow \quad C_3 + C_4 = 0 \quad \boxed{C_3 = -C_4}$

@ $\bar{y}=1,\ Y=0$

$$\Rightarrow \quad Y(\bar{y}) = C_3\left[e^{(n^2\pi^2-Da)^{1/2}\bar{y}} + e^{-(n^2\pi^2-Da)^{1/2}\bar{y}}\right]$$

$$\Rightarrow \quad 0 = C_3\left[e^{(n^2\pi^2-Da)^{1/2}} - e^{-(n^2\pi^2-Da)}\right]$$

$c.$

$$Y = C_1 \sinh[(n\pi)^2 - Da)\bar{y}]$$

Now; $\quad \bar{C} = X(\bar{x}).Y(\bar{y})$

$$\bar{C} = \Sigma C_n \sin(n\pi\bar{x}).\sinh[(n\pi)^2 - Da)\bar{y}]$$

at $\bar{x}=1$

$\bar{C} = \frac{C}{C_m}$

$\left(\bar{C} = \frac{f(x)}{C_m}\right)$

$$\frac{f(x)}{C_m} = \Sigma C_n \sin(n\pi\bar{x}).\sinh[(n\pi)^2 - Da)\bar{y}]$$

$$C_n = \int \frac{f(x).\sin(n\pi\bar{x})}{C_m \sin(n\pi\bar{x})^2 \sinh[(n\pi)^2 - Da)\bar{y}]} d\bar{x}$$

$$\boxed{C = \Sigma C_m \sin\left(\frac{n\pi x}{L}\right).\sinh\left[\left((n\pi)^2 - Da\right)\frac{y}{L}\right]}$$

Date - 03 April

(B) FD → Finite difference }
F.E → Finite element }.

Finite element → Approximate soln (COMSOL, ANSYS)
Finite difference → Approximate the governing eqn.

FEM → finite element method

$$\boxed{\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - K} \quad (1)$$ (one D, zeroth order rxn)

(→ we need to go approximate the governing eqn. because domain is not always fixed geometry)

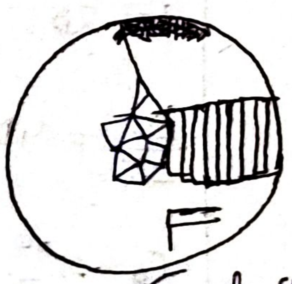
→ difficult to find out the IC & BC.

→ FEM discretise the domain in small domain and eq (1) represents the global eqn.

→ Global eqn.

Consider a simple geometry.

circle.



Steps

→

→ coordinate axes. (local coordinates) (Global eqn → local coordinate system)

→ $$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - K$$

$t = \frac{L}{V_{...}} = \frac{x}{V}$

→ $\frac{\partial c}{\partial}$

(Interpolation)

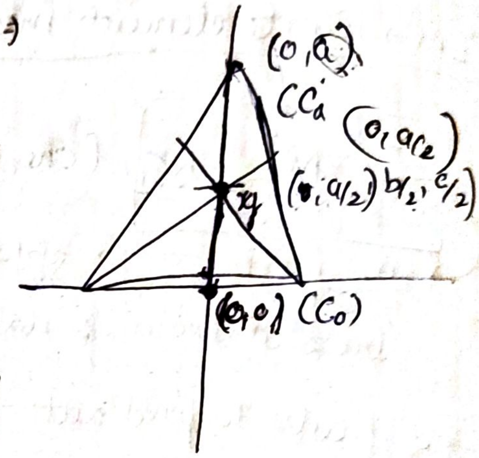
Interpolation

$x = \frac{a+b}{2} = \frac{h}{2}$

$$\frac{\partial c}{\partial t} = D\left(\frac{\partial^2 c}{\partial x^2}\right) - K$$

$$\frac{\partial C}{\partial t} = 4D\frac{\partial^2 c}{\partial x^2} - K$$

$$\frac{dc}{dt} = \frac{C(a) - C(b)}{\Delta t} = \frac{C(a) - C(b)}{\Delta t}$$



2(ca interpolation

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 c}{\partial y^2} - K$$

$$\frac{\Delta C}{\Delta t} = 4D\left(\frac{\partial^2 c}{\partial a^2} + \frac{\partial^2 c}{\partial b^2} + \frac{\partial^2 c}{\partial c^2}\right) - K$$

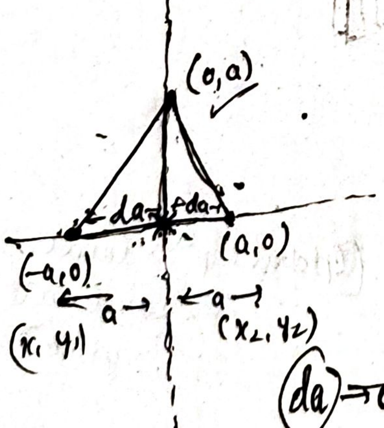
$$\frac{\Delta C}{\Delta t} = 4D\left[\frac{\partial^2 c}{\partial a^2} + \frac{\partial^2 c}{\partial b^2} + \frac{\partial^2 c}{\partial c^2}\right] - K$$

For 2D

$$\frac{\Delta C}{\Delta t} = 4D\frac{\partial^2 c}{\partial a^2} - K$$

$$\frac{C_a - C_0^{\to 0}}{\Delta t} = 4D\frac{\partial^2 c}{\partial a^2} - 4K$$

$$C_a = \Delta t\left(4D\frac{\partial^2 c}{\partial a^2} - 4K\right)$$



$$f = \sqrt{s(s-a)(s-b)(s-c)} \qquad \left(s = \frac{a+b+c}{2}\right)$$

or. Area.

$\frac{2a-a+b-c}{2}$

$f = \cancel{\sqrt{\left(\frac{a+b+c}{2}\right)\left[\frac{a-b-c}{2}\right]\left[\right.}}$

$\frac{a+b+c-}{2}$

$$f^2 = \left(\frac{a+b+c}{2}\right)\left[\frac{b+c-a}{2}\right]\left[\frac{a+c-b}{2}\right]\left[\frac{a+b-c}{2}\right]$$

$$f^2 = \frac{\left[(a+b+c)(b+c-a)(a+c-b)(a+b-c)\right]}{16}$$

$$g^2 = \frac{3 \cdot 14 \; u}{\rho g}$$

$d = r_H = \frac{1}{4}\delta$

$r_H = 4\delta$

$$25 = N_u = \frac{8 \cdot 14 \cdot 84}{4u}$$

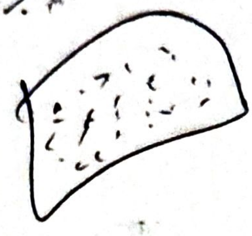
$$\boxed{\varnothing\ \frac{1}{g} = \frac{25 \times 4u}{4\rho \delta}}$$

$g^2 \rightarrow$

$1 \rightarrow \tau$

$n a \rightarrow n\tau$

Flux $\rightarrow \frac{kg}{m^2\, sec} \times \frac{mol/m^3}{m}$



$\frac{m^2}{s}$

$\tau \rightarrow$

total time $\rightarrow t =$ ~~speed~~ $\left(\frac{\text{distance}}{\text{speed}}\right) \times l.$

$x_n l.$ $\quad t =$ ~~speed~~

$=$

$=$

$D =$