

Mass Transfer

- Chemical Potⁿ is the driving force behind mass transfer that occurs through diffusion.

Diffusion

Molecular Diffusion

Only due to KE of molecules

Ex - sugar diffusing into a cup of tea on its own

Eddy Diffusion

This is convective mass transfer when eddy currents are created by a convective velocity field by some external force.

Ex - sugar diffusing into tea after stirring.

- Velocity enhances diffusion since it breaks down the fluid into smaller fragments and hence there is less resistance due to less energy & this expedites the process.

\rightarrow O_2 Net moment \rightarrow

$\begin{array}{ccccccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{array}$

Mean path \downarrow

mechanical separation or techniques
The difference between physical separation the former is based
and mass transfer is that size, shape etc. while
on physical factors like size, shape etc. while
the latter is based on p.

Terms

molal conc'

concentration is denoted in two ways \rightarrow molal conc'

$$\left. \begin{array}{l} \rho_i \rightarrow \text{density} \rightarrow \frac{\text{mass}}{\text{volume}} \\ w_i \rightarrow \text{mass fraction} \end{array} \right\} \text{mass conc}'$$
$$w_i = \frac{\rho_i}{\sum \rho_i}$$

c_i used for molal conc'

$$\left. \begin{array}{l} \alpha_i \rightarrow \text{solid phase mole fraction} \\ \gamma_i \rightarrow \text{vap. f.} \end{array} \right\} \text{size } \Sigma \gamma_i = 1$$

Average velocity

component velocity $\rightarrow \bar{u}_i^o$

- When the weight used is ρ_i^o , \bar{u} is called molar average velocity and is denoted by U .
- When the weight used is ρ_i^o , \bar{u} is called mass average velocity and is denoted by \bar{u} .

$$U = \frac{\sum u_i \rho_i^o}{\sum \rho_i^o} \quad & \bar{u} = \frac{\sum \bar{u}_i \rho_i^o}{\sum \rho_i^o}$$

$$\boxed{U = \frac{\sum u_i \rho_i^o}{\sum \rho_i^o}} \quad & \boxed{\bar{u} = \frac{\sum \bar{u}_i \rho_i^o}{\sum \rho_i^o}}$$

Mass Flux

Molar Flux

$$N_i^o$$

$$\text{Rel. vel.} = 0$$

$$N_i^o = \bar{u}(u_i^o - 0) \quad J_i^o = \bar{u}(u_i^o - 0)$$

$$N_i^o = \rho_i^o(u_i^o - 0)$$

$$J_i^o = \rho_i^o(u_i^o - U)$$

$$\bar{u}^o = \rho_i^o(u_i^o - U)$$

Mass Flux

$$\boxed{J_i^o = \bar{u}(u_i^o - U)}$$

$$\boxed{F_i}$$

$$\boxed{- J_n}$$

$$\boxed{J_n}$$

J_i is called diffusive flux and N_i is called total flux

def

relationship between J_i and N_i

$$J_i = \frac{c_i u}{c_u} \quad N_i = c_i u$$

$$u = \frac{\sum c_i u}{\sum c_i}$$

u

total diffusive flux

$$J_t = N_t = \frac{c_e}{c_u} \sum N_i$$

total flux conervative flux

Flux

$$J_A = -\frac{dc_A}{dx}$$

Fick's law

- In molecular diffusion, chemical potential is equal to driving force and there is no diff.

We use J since we only want to capture molecular diffusion \Rightarrow only due to molecular motion

$$J_A \propto -\frac{dc_A}{dx}$$

$$\Rightarrow J_A = -D_{AB} \frac{dC_A}{dx}$$

\Rightarrow

D_{AB} is called diffusivity of A in B and usually depends on B

- Dimension of D_{AB} is $\frac{m^2}{s}$ & SI unit is

Fick's law in terms of N_A

$$J_A = N_A - \frac{C_A}{C} (N_A + N_B) = -D_{AB} \frac{dC_A}{dx}$$

Q. Prove that for binary system at constant temp. and pressure, $D_{AB} = D_{BA}$

$$\begin{aligned} C &= C_A + C_B \\ \Rightarrow \frac{dC_A}{dx} &= \frac{dC_A}{dx} + \frac{dC_B}{dx} \end{aligned}$$

$$\Rightarrow \boxed{\frac{dC_A}{dx} = -\frac{dC_B}{dx}} \quad (1)$$

$$\begin{aligned} J_A &= N_A - \frac{C_A}{C} (N_A + N_B) \\ J_B &= N_B - \frac{C_B}{C} (N_A + N_B) \end{aligned} \quad \left\{ \begin{array}{l} \text{2)} J_A + J_B = N_A + N_B \\ \text{2)} - (N_A + N_B) \end{array} \right.$$

$$\boxed{J_A + J_B = 0}$$

Also, by Fick's law, $-J_A = \frac{-dC_A}{dx} \cdot D_{AB} \cdot \Delta P$

$$\& J_B = -\frac{dC_B}{dx} \cdot D_{BA}$$

$$1) J_A + J_B = 0 \Rightarrow -\frac{dC_A}{dx} \cdot D_{AB} = -\frac{dC_B}{dx} \cdot D_{BA}$$

$$\Rightarrow D_{AB} = D_{BA} \quad (\text{from } ①)$$

Chemical Pot^n

Fick's law on terms of pressure at constant temp. and diff. at diff.

$$\text{We know, } \mu_A = \mu_0 + RT \ln \gamma_A + RT \ln(C_A)$$

$$2) \frac{d\mu_A}{dx} = \frac{RT}{C_A} \frac{dC_A}{dx}$$

$$\text{Fick's law} \rightarrow J_A = -D_{AB} \cdot C_A \frac{d\mu_A}{dx} = -\frac{D_{AB} \cdot C_A}{R \cdot T} \frac{d\mu_A}{dx}$$

* Heat, mass and momentum transfer are analogous to each other. Thermal diffusivity = $\frac{k}{\rho C_p}$
 Mass diffusivity $D_{AB} = \alpha = \frac{\rho}{\eta} \rightarrow$ momentum diffusivity $\approx \frac{H}{\eta}$ (dynamic viscosity)

(NB) $\boxed{5}$

Heat Transfer

$$q = -k \cdot \frac{dT}{dx}$$

Fourier's law

$$\dot{q} = -\left(\frac{k}{\rho C_p}\right) \cdot \frac{d(pT)}{dx}$$

↓ same dimensions

Mass Transfer

$$\dot{m}_A = -D_{AB} \cdot \frac{dx}{dx} \cdot \text{concn.}$$

Momentum Transfer

$$T = -H \frac{dv}{dx}$$

Newton's Law

$$T = -H \int \frac{dv}{dx}$$

Pressure Gradient

$$\therefore \alpha = D_{AB} \equiv \frac{H}{P}$$

Binary Diffusivity

Theories and Correlation

Solid Diffusivity (Surface)

→ Pore diffusion → Knudsen Diffusivity

• Kinetic Theory

(No intermolecular forces)

• Lattice Model

• Statistical

• Molecular

Gas Diffusivity liquid Diffusivity

1. Kinetic Theory

(No intermolecular forces)

2. Modified kinetic

3. Theorie der

Stoer Potential

to evaluate the force

- Hirschfelder et al
 (same as Chapman)
 and by Enkong)

3. Fuller, Schettler and
Giddings - reliable
when "parameters are
not accurate"

4. Others

Non Polar and non reacting

and hydrodynamical

→ 1. Eyring's theory

theory

Fuerstlin eq

2. Smakler - Fuerstlin eq

• mostly for colloidal soln

• explains the dependence of viscosity & T.

3. Wilke Chong for dil. soln

4. Hafclund & Landolt

• for infinite dilution
correlation for conc

Gas Diffusivity

- Mainly governed by

i) Kinetic Theory
ii) Modified Kinetic Theory

- According to kinetic theory self-diffusion coefficient of A, D_{AA} is given by

$$D_{AA} = \frac{1}{3} \lambda H \quad (1)$$

$$\lambda = \frac{K T}{\sqrt{\pi n \sigma_A^2 p}} \quad (2)$$

$$H = \sqrt{\frac{8 k N T}{\pi M_A}} \quad (3)$$

A → mean free path
 $H \rightarrow$ mean speed

K → boltzmann const.
N → Avogadro no.

σ_A → diameter of spherical molecule.

M_A → Mol wt. of A

- Combining (1), (2) and (3) we get

$$D_{AA} = \frac{2}{3} \cdot \left(\frac{K}{\pi} \right)^{3/2} \cdot N^{1/2} \cdot T^{3/2} \cdot \left[\frac{\left(\frac{1}{M_A} \right)^{1/2}}{P \sigma_A^2} \right]^{1/2} \quad (4)$$

$$D_{AB} = \frac{2}{3} \cdot \left(\frac{K}{\pi} \right)^{3/2} \cdot N^{1/2} \cdot T^{3/2} \cdot \left[\frac{\left(\frac{1}{M_A} + \frac{1}{M_B} \right)^{1/2}}{P \left(\frac{\sigma_A}{2} + \frac{\sigma_B}{2} \right)^2} \right]^{1/2} \quad (5)$$

Eg ⑤
for

CO_2

Eq ⑤

Chapman

Eg

Here

is applicable for ideal gas where "internal forces" are not accounted for,

$$\text{Eq}^1 \quad \frac{\sigma_A + \sigma_B}{2} \quad \text{and} \quad \left(\frac{1}{M_A}\right)_{\text{av}} = \frac{1}{2M_A} + \frac{1}{2M_B}$$

⑤ only applicable when A & B are very close to each other,

Chapman and Enskog

$$\phi(r) = 4e^{-\left[\left(\frac{\sigma}{r}\right)^{12} + \left(\frac{\sigma}{r}\right)^6\right]}$$

where $\phi(r)$ = derjard-Jones potential function

σ = distance b/w the centres of two molecules

$e \& \sigma$ = Lennard-Jones potential parameters

$$\text{Eq}^1 \rightarrow D_{AB} = \frac{1.858 \times 10^{-7} \cdot T^{3/2} \left(\frac{1}{M_A} + \frac{1}{M_B} \right)^{1/2}}{(m^2/s)}$$

Here, T = absolute temp., in K
 M_A, M_B = Mol wt of A & B
 P = Total pressure

5

σ_{AB} = a characteristic length parameter of factors

in the binary

$\sqrt{\nu_D}$ = collision integral which is a function of

$$\frac{kT}{E_{AB}}$$

$$\sigma_{AB} = \frac{\sigma_A + \sigma_B}{2}$$

$$E_{AB} = \sqrt{e_A e_B}$$

V_L = molar volume at normal BP (cm³)

$$\begin{aligned} \frac{e}{k} &= 0.77 \frac{T_c}{T} \text{ and } \sigma = \frac{5}{6} (V_L)^{1/3} \\ K &= 1.15 T_c (\text{normal BP}(K)) = 1.18 V_L^{1/3} \\ &= 2.44 \left(\frac{T_c}{P_c} \right)^{1/3} \end{aligned}$$

Fuller Correlation

$$D_{AB} = 10 \times T^{1.75} \left(\frac{1}{M_A + M_B} \right)^{1/2} P \left[\left\{ \frac{(\sum v)}{V} \right\}_A^{1/3} + \left\{ \frac{(\sum v)}{V} \right\}_B^{1/3} \right]^2$$

$$\text{where } v = \text{atomic volume, } \sum v = V_c + 4 \times V_H$$

P = Total pressure in atm

T = Temp. in K

factors affecting gas phase diffusivity

of

temp.

pressure

molar wt.

at normal
BPP (cm³)

any other parameter which affect intermolecular
non-ideality such as chemical nature.

Any other non-idealities such as chemical nature.

intermolecular force

$$\frac{D_{AB} T_1}{D_{AB} T_2} = \left(\frac{T_1}{T_2} \right) \cdot \left(\frac{P_2}{P_1} \right) \cdot \left(\frac{N_2 D_2}{N_1 D_1} \right)$$

where you neglect intermolecular forces

$$P_2 = P_1$$

$$and \quad D_{AB} = P \left(\frac{K T}{C_{AB}} \right)$$

Multicomponent diffusion

$$D_{im}^o = N_i^o - \frac{Y_i \sum_{j=1}^n N_j^o}{\sum_{j=1, i \neq j}^n D_{ij}^o (Y_j^o N_i^o - Y_i^o N_j^o)}$$

where D_{im} is the
diffusivity of i^o
in mixture

Special Case

If only A is diffusing and all other components
are non-diffusing

$$D_{AM} = \frac{\eta}{\sum_{i=2}^n \frac{y_i}{D_{Ai}}} = \frac{y_2}{D_{A2}} + \frac{y_3}{D_{A3}} + \dots$$

- consider a mixture of gas with comp' A, B, C & D.

The diffusion of A in mixture is still governed by Fick's law by replacing the diffusivity by D_{AM} .

$$J_A = - D_{AM} \frac{dy_A}{dx}$$

$$\text{and } D_{AM} = \frac{1}{\frac{y_B}{1-y_A} + \frac{y_C}{1-y_A} + \frac{y_D}{1-y_A}}$$

Wink

- comb

Liquid Phase Diffusivity

- No reliable theory is available
- Limited correlations are available
- Not as accurate as to gas phase diffusivity
- Eyring's theory and ~~hydrodynamic~~ hydrodynamic

Two commonly used theories:
 theory → Smoluchowski and Einstein eqⁿ

Hydrodynamic theory
 based on hydrodynamics so that $H \approx H_B$
 valid for dil. soln so that $H \approx H_B$
 Valid for $r \gg R_A$ or $r \rightarrow \text{radius of } A$

$$D_{AB} = \frac{kT}{6\pi\eta H_B}$$

$$\boxed{\frac{D_{AB} H_B}{T} = \text{constant}}$$

Witke-Chang Correlations

- combining Eyring and Hydrodynamic theory

$$\frac{D_{AB} H_B}{T} = f(V_A)$$

$$\Rightarrow \boxed{\frac{D_{AB} H_B}{T} = \frac{7.4 \times 10^{-8} (\phi_B M_B)^{1/2}}{24 V_A^{0.6}}} \quad \begin{cases} D_{AB} \text{ in } \text{cm}^2/\text{s} \\ \phi_B \text{ in volume} \end{cases}$$

ϕ_B = Association factor
 V_A = $0.985 V_C$ where V_C is ~~initial~~ volume
 (if data not available)

$$* \frac{D_{AB} M_B}{T} = \frac{1.173 \times 10^{-16} (\phi_B M_B)^{1/2}}{M_D^{0.6}} \quad \text{where all SI units}$$

- It is also based for very dil. soln.
- Hayduk & Laudil Correlation → used for "pure" solutions
- Correlation factors for concentration

$$D_{AB}^{\circ} = 13.26 \times 10^{-5} \times M_B^{-1.14} \times T^{0.589}$$

$$\& D_{AB,M}^{\circ} = (D_{AB}^{\circ} \times M_B) X_B (D_A \cdot M_A) X_A$$

Factors affecting liquid phase Diffusivity

- Temperature
- Viscosity
- conc'
- Mol. wt. (chemical nature)
- Solvent, solute "inert" parameter

Pore (Knudsen) Diffusion

- The diffusion of molecules within pores or microchannels
- where pore / channel diameter $< \lambda = \text{K number}$

If diameter of pore $> \lambda$ = molecular diffusion
(no restriction by pore)

If pore $< \lambda$ = pore diffusion
(pore restricts the motion)

$K_n > 1$ = Knudsen diffusion

$$K_n = \frac{\lambda}{d}, \quad K_n < 1 = \text{molecular}$$

Knudsen no.

Pure Knudsen diffusion

Cylindrical channel

$$J_A = D_{KA} \left(\frac{\rho}{\tau} \right) \frac{dC_A}{dx}$$
$$J_A = \text{Diff.} \cdot \frac{dC_A}{dx}$$

$$\frac{L}{L'} = \frac{1}{\tau}$$

* \rightarrow Tensionality, A and $\epsilon \rightarrow$ porosity

How to estimate D_{KA}

$$- D_{AA^*} = \frac{1}{3} H$$

homogeneous

- Conse → RA → Rate
- * $D_{KA} = \frac{dp_{pure} \cdot H}{3} = \sqrt{\frac{8\pi N T}{\pi M A}}$
- $D_{KA} = 4857 dp_{pure} \sqrt{\frac{T}{M A}}$
- where D_{KA} → Pure Knudsen diffusion, no molecular diff.
- * Knudsen diffusion along with molecular diffusion
- $J_A = D_{eff}' \cdot \frac{dy_A}{dx}$
- $D_{eff}' = D_{KA} \cdot \frac{e^2}{T} \text{ or } D_{KA} \cdot e^2$
- where $\frac{1}{D_{eff}'} = \frac{1 - \alpha y_A}{D_{AB}} + \frac{1}{D_{KA}}$
- where $y_A = \text{mole fraction}$
- $\alpha = 1 + \frac{N_A}{N_B}$
- when $N_A = N_B$ or $y_A \sim 0 \Rightarrow \alpha \sim 1$, we get
- $\frac{1}{D_{eff}'} = \frac{1}{D_{AB}} + \frac{1}{D_{KA}}$
- 2) When $N_A \gg N_B$ or $y_A \sim 1$, then no molecular diffusion
- Specia → - Specia
- Specia → - Specia
- Specia → - Specia

Conservation of mass in terms of flux

rate of moles of A generated per unit volume
 $\rightarrow R_A$

Rate of mass of ($\text{in} - \text{out} + \text{accumulation} - R_A$)

molecular
diff.

fluxion

$$\begin{aligned} \text{Rate of in} &\rightarrow N_A |\chi \Delta y \Delta z - N_A |\chi_{\text{ext}} \Delta y \Delta z \\ \text{Rate of out} &\rightarrow N_A |\chi y \Delta z - N_A |\chi_{\text{ext}} y \Delta z \\ &+ N_A |\chi y \Delta y - N_A |z + \Delta z \Delta x \Delta z \\ &+ N_A |z \Delta x \Delta y - N_A |z + \Delta z \Delta x \Delta y \\ \text{Rate of acc} &= \frac{d}{dt} \left(\Delta x \Delta y \Delta z \frac{P}{N_A} \right) \quad \text{at } u \frac{d}{dt} (\text{mole}) \end{aligned}$$

Rate of gen' $\rightarrow R_A \cdot \Delta x \Delta y \Delta z$

$$2) \frac{\delta N_A}{\delta x} + \frac{\delta N_A}{\delta y} + \frac{\delta N_A}{\delta z} = \overline{R_A}$$

$\sim 1,$

no
molar
concen-

- Steady state (~~at equilibrium~~ accumulation = 0)
- No gen' ($R_A = 0$)
- One -D

$$\text{Then } \frac{\partial N_A}{\partial x} = 0 \Rightarrow [N_A = \text{constant}]$$

- for variable geometry i.e. $A|_x \neq A|x + \Delta x$

$$\boxed{\frac{d}{dt}(A, N_A) = 0}$$

Fick's Second Law

We know,

$$\frac{dN_A}{dx} = 0 \quad \text{for steady state, no reaction}$$

const area

$$\Rightarrow \frac{d}{dx} \left[J_A + \frac{C}{C} (N_A + N_B) \right] = 0 \quad (1 - D)$$

Under "no", when $N_A = -N_B$
and $C_A \approx 0$

$$\Rightarrow \frac{d}{dx} (J_A) = 0$$

$$\Rightarrow \frac{d}{dx} \left(-D_{AB} \frac{\partial N_A}{\partial x} \right) = 0$$

$$\Rightarrow \boxed{\frac{d^2 N_A}{dx^2} = 0}$$

Molecular Diffusion Analysis

case 1 → binary, non-reactive, steady state, constant geometry
 $A \uparrow, B \uparrow, N_A = 0$

Single phase

$$x = l, C_A = C_{A1}$$

$$N_A = 0, C_A = C_{A1}$$



$$\text{Fick's law} \rightarrow J_A = -D_{AB} \frac{dC_A}{dx}$$

$$\Rightarrow N_A = -\frac{CA}{C} (N_A + N_B) = -D_{AB} \frac{dC_A}{dx}$$

$$\text{Flux conservation} \rightarrow \frac{dN_A}{dx} = 0$$

$$\Rightarrow N_A = -\frac{N_A \frac{CA}{C}}{C} + D_{AB} \frac{dCA}{dx}$$

$$\Rightarrow N_A dx = -\frac{D_{AB} dCA}{C - CA_1}$$

$$\Rightarrow N_A \int_0^l dx = -D_{AB} C \int_0^l \frac{dCA}{C - CA_1}$$

$$\Rightarrow N_A = \frac{D_{AB} C}{l} \ln \frac{C_{A1} - C}{C_{A1} - C}$$

Case
binary
vap

Mass, $C = C_{A_1} + C_{B_1}$
 $= C_{A_2} + C_{B_2}$

Let $\text{concn} = \frac{C_{B_2} - C_{B_1}}{\ln \frac{C_{B_2}}{C_{B_1}}} = \frac{C_{A_1} - C_{A_2}}{\ln \frac{C_{A_1}}{C_{A_2}}}$

$$\therefore N_A = \frac{D_{AB} C}{l \ln \text{concn}} \cdot \frac{C - C_{A_1}}{C - C_{A_2}} \times \frac{C_{A_1} - C_A}{C_{A_1} - C_{A_2}}$$

$$N_A = \boxed{\frac{D_{AB} C}{l \ln \text{concn}} \cdot (C_{A_1} - C_{A_2})}$$

$$\star N_A = \boxed{\frac{D_{AB} C}{l C_B \ln l} (C_{A_1} - C_{A_2})}$$

It is called Mass transfer coefficient or flux = $N_A C \times D$

* concn profile at any x , $y_A = \frac{C - C_A}{C - C_{A_1}} = \boxed{M \left(\frac{C - C_{A_2}}{C - C_{A_1}} \right)}$

* $y_A = \frac{C_{A_1}}{C} \quad \& \quad y_B = \frac{C_{A_2}}{C}$

Case II

non-reactive, steady state, single phase,
binary geometry
and first order diffusion

$A \uparrow B \downarrow$

when $\alpha = 1$ i.e. equimolar

$$\text{det } N_A = -x N_B \quad 0$$

$$N_A - \frac{c_A}{c} (N_A + N_B) = -DAB \frac{\text{det}}{dx}$$

and $N_A = \text{constant}$

$$N_A = -N_B$$

$$\Rightarrow N_A = -DAB \int \frac{dc_A}{dx}$$

$$N_A = DAB \left(\frac{c_{A_1} - c_{A_2}}{l} \right)$$

$$\frac{dN_A}{dx} = 0, \text{ i.e. } c_A = \frac{C_A}{DAB} x + C_2$$

$$N_A = \frac{DAB C}{l} \left[\frac{x_{A_1} - x_{A_2}}{x_{B_{lm}}} \right]$$

* For gas,

$$N_A = \frac{D_{AB} C}{L} \left[\frac{y_{A_1} - y_{A_2}}{(y_B) \text{ km}} \right]$$

$$= \frac{D_{AB} P}{RT L} \left[\frac{P_{A_1} - P_{A_2}}{(P_B) \text{ km}} \right]$$

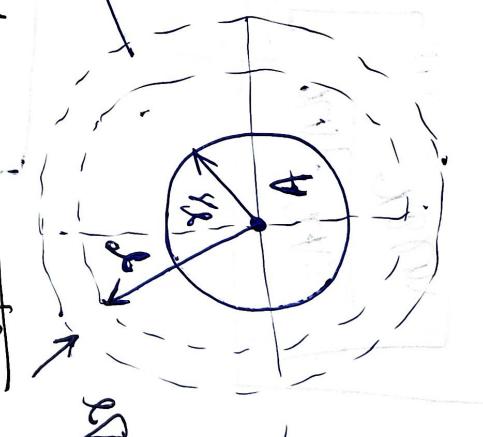
For liquid,

$$N_A = \frac{D_{AB} C}{L} \left[\frac{x_{A_1} - x_{A_2}}{(x_B) \text{ km}} \right]$$

$$\boxed{\frac{C - C_A}{C_A - C_{A_2}} = \frac{2}{L}}$$

* Concentration profile for equimolar \rightarrow

Diffusion in Spherical Geometry



This is a binary system of water vap(A) through air(B).

Rate of transport of A into the thin shell (at $r=R$)

$$= (4\pi r^2) N_A |_{r=R}$$

Rate of output of A from the tank shell
(at $r = r + \Delta r$) = $(4\pi r^2) N_A |_{r+\Delta r}$

Steady-state mass balance,

$$(4\pi r^2) N_A |_r + (4\pi r^2) N_A |_{r+\Delta r} = 0$$

(Input) (Output)

Dividing both sides by Δr and taking the limit
 $\Delta r \rightarrow 0$

$$\lim_{\Delta r \rightarrow 0} \frac{(4\pi r^2) N_A |_r - (4\pi r^2) N_A |_{r+\Delta r}}{\Delta r} = 0$$

$$2) - \frac{d}{dr} (4\pi r^2 N_A) = 0$$

$$2) N_A \cdot 4\pi r^2 = \text{const.} = W(\text{say})$$

* In general for steady state diffusion,

$(\text{Area})(\text{Flux}) = \text{constant}$

$r = d$

$$\text{Now, } N_A = (N_A + N_B) \frac{c_A}{c} - D_{AB} \frac{dc_A}{dr}$$

$$\Rightarrow N_A \left(\frac{c - c_A}{c} \right) = - D_{AB} \frac{dc_A}{dr}$$

$$\Rightarrow N_A \approx - \frac{D_{AB} C}{c - c_A} \frac{dc_A}{dr}$$

$$\Rightarrow \frac{W}{4\pi r^2} = - \frac{D_{AB} C}{c - c_A} \cdot \frac{dc_A}{dr}$$

$$\Rightarrow \int_{c_A}^{c} \frac{-dc_A}{c - c_A} = \frac{W}{4\pi r^2} \int_{r_1}^{r_2} \frac{dr}{r^2}$$

~~$$\Rightarrow \int_{c_A}^{c} \frac{-dc_A}{c - c_A} = \frac{W}{4\pi r^2} \int_{r_1}^{r_2} \frac{dr}{r^2}$$~~

$$W = (4\pi D_{AB} C) \ln \frac{c - c_A}{c_A}$$

- * W is the constant molar rate of mass transfer so it is equal to the rate of "rap" of the drop at any instant

$$W = -\frac{d}{dt} \left(\frac{4\pi r_8^3}{3} \frac{\rho_A}{M_A} \right) = -4\pi \frac{\rho_A}{M_A} \cdot \frac{dr_8}{dt}$$

$$\Rightarrow -4\pi \frac{\rho_A}{M_A} \cdot \frac{dr_8}{dt} = (4\pi D_{AB} C) \ln \frac{C - CAx}{C - CAx(t)}$$

$$\Rightarrow -r_8' \int r_8 dr_8 = \frac{D_{AB} CM_A \ln \frac{C - CAx}{C - CAx(t)}}{\rho_A}$$

$r_8 = r_{80}$ and

assuming $t=0$, radius of drop is r_{80} and
 $t=t'$

$$\Rightarrow r_{80}^2 - r_8'^2 = \frac{2D_{AB} CM_A t'}{\rho_A} \ln \frac{C - CAx}{C - CAx(t')}$$

* time for "complete envelop" when $r_8' = 0$,

$$t' = \frac{\rho_A r_{80}^2}{2D_{AB} CM_A \ln [(C - CAx) / (C - CAx(t'))]}$$

* brittle cylinder case from book (Pg. 52)

after

Diffusion through a tapered tube

Pg. 54

Depletion Time (Binary steady state)

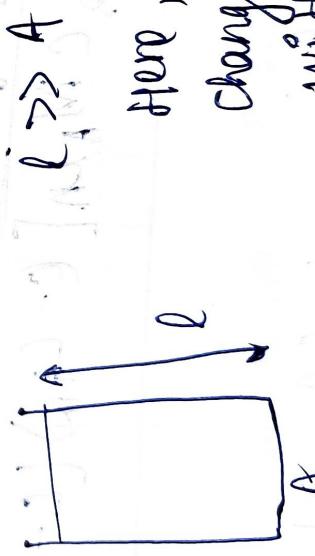
Case - 1 → ~~different~~ diffusional surface area is large compared to depth

$$t = \frac{A_d \frac{s_A}{N_A}}{N_A}$$

A diagram of a rectangular tube with length labeled l and cross-sectional area labeled A .

Basically amount present flux
 $A \gg l$

Case 2 → Diffusional surface area is small compared to depth



Here, N_A will change as l will significant change over time with time

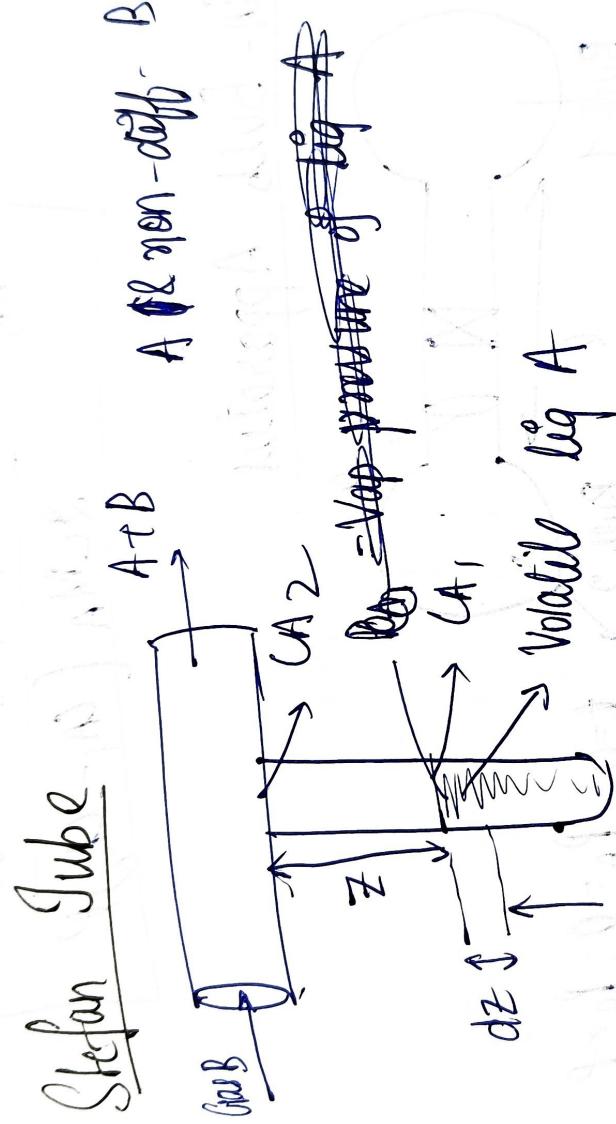
$$N_A = \frac{DAB C}{L} (C_{A_1} - C_{A_2})$$

$$N_A \cdot A = \frac{DAB}{L} (C_{A_1} - C_{A_2})$$

Measurement of Diffusivity (Experimental methods)

Gas Phase → Stefan tube / Arnold cell
 → Twin bulb method
 → Diaphragm cell (similar to Twin bulb method)
Liquid Phase → Diaphragm bulb method

Stefan tube



$$N_A = \frac{D_{AB} C (C_{A1} - C_{A2})}{z (C_{A1})}$$

If fall in the liquid level is dz in a small time dt , the no. of moles A that diffuses out is $dN_A = \frac{dA}{M_A} dt$. By a material balance over

$$\frac{adz \rho_A}{M_A} = ad_A dt = \frac{adABC(C_1, C_2)}{Z(z_{0m})} \cdot dt$$

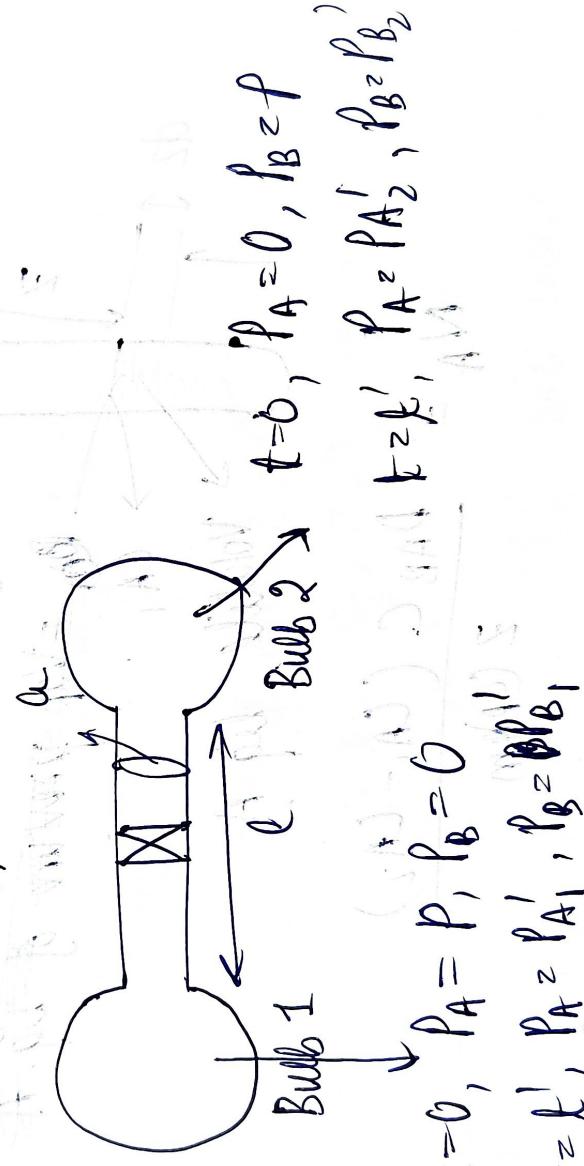
where a is inner cross section of the tube.

$$t \rightarrow t=0, z_0$$

$$t = t^1, z^1$$

$$D_{AB} = \frac{(C_B) \ln \rho_A (z^1)^2 - z_0^2}{2CMA(C_1 - C_2)t^1}$$

Twin-Bulb Apparatus



$$t=0, P_A = P, P_B = 0$$

$$t = t^1, P_A = P_A^1, P_B = P_B^1$$

$$\text{Ansatz: } \frac{adABC(P_A^1 - P_A^2)}{RTL} = - \frac{\partial P_B}{\partial t}$$

If C_1 and C_2 are the instantaneous conductances of A in the bulbs, the rates of change are

$$-V_1 \frac{dCA_1}{dt} = \alpha N_A \Rightarrow -\frac{V_1}{RT} \frac{dPA_1}{dt} = \alpha N_A$$

$$-V_2 \frac{dCA_2}{dt} = \alpha N_A \Rightarrow -\frac{V_2}{RT} \cdot \frac{dPA_2}{dt} = \alpha N_A$$

$$\begin{aligned} \Rightarrow -\frac{d}{dt} (PA_1 + PA_2) &= \alpha RT \left(\frac{1}{V_1} + \frac{1}{V_2} \right) N_A \\ &= \frac{\alpha PA_{AB} (PA_1 - PA_2)}{Q} \left(\frac{1}{V_1} + \frac{1}{V_2} \right) \end{aligned}$$

$$\Rightarrow -\frac{d}{dt} (PA_1 - PA_2) = \frac{\alpha DA_{AB}}{Q} \left(\frac{1}{V_1} + \frac{1}{V_2} \right) dt$$

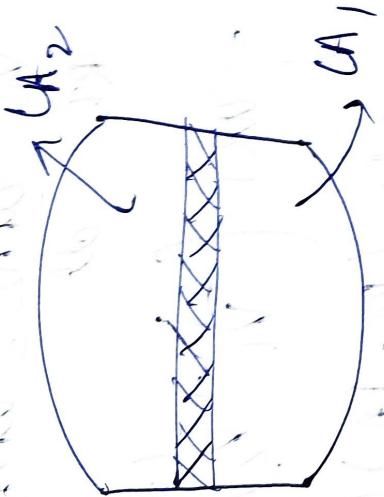
$$\begin{aligned} t=0, \quad PA_1 - PA_2 &= P - 0 = P \\ t=t', \quad PA_1 - PA_2 &= PA'_1 - PA'_2 = PA_1 - PA_2' \end{aligned}$$

$$\ln \frac{P}{PA'_1 - PA'_2} = \frac{\alpha DA_{AB}}{Q} \left(\frac{1}{V_1} + \frac{1}{V_2} \right) t'$$

P_{B2}

Ans

Diaphragm cell



A is the area of diaphragm
 ϵ is its porosity
a.e. is effective area

The pores may not be straight, so

$$\text{eff. porosity} = \frac{\text{avg length of diff.}}{\text{thickness of chap.}}$$

Con-

$$NA = -D_{AB} \frac{dC}{dz}$$

$$2) NA = \frac{D_{AB}(CA_1 - CA_2)}{kT}$$

Effusive length
l is thickness of diaphragm

$$\text{Now, } -V_1 \frac{dCA_1}{dt} = \alpha e N_A \quad \& \quad V_2 \frac{dCA_2}{dt} = \alpha e N_A$$

$$-\frac{d}{dt}(CA_1 - CA_2) = \alpha e D_{AB} \frac{(CA_1 - CA_2)}{lT} \cdot \left(\frac{1}{V_1} + \frac{1}{V_2} \right)$$

initial concentrations

if C_{A10} and C_{A20} are initial and C_{A1f} and C_{A2f} are final
and $\frac{1}{\alpha} \epsilon k_p$ and $\frac{1}{\alpha} \epsilon k_p \left(\frac{1}{V_1} + \frac{1}{V_2} \right) \ln \left(\frac{C_{A1,0} - (C_{A2,0})}{C_{A1,f} - (C_{A2,f})} \right)$

$$\text{then } \frac{\alpha \epsilon}{\tau L} \left(\frac{1}{V_1} + \frac{1}{V_2} \right) = \beta$$

Here

of diff.
of chap.

Convective Mass Transfer

The constants of proportionality k_p, K_c & K_f are

Here, $N_A = K_c \cdot \Delta C_A$ { say Δy_A }
 $\therefore N_A = K_f \cdot \Delta P_A$ { say ΔP_A }

$$N_A = K_c \cdot \Delta C_A \quad \text{liquid}$$
$$= K_f \cdot \Delta x$$

$$\left(\frac{1}{V_1} + \frac{1}{V_2} \right)$$

* Unif

$$\rightarrow K_f = K_c = m/s$$

$$K_m = K_f = \text{mol/m}^2 s$$

$$K_f = \text{mol/m}^2 s$$

$$K_c = RT K_f \Rightarrow \boxed{K_f = \frac{K_c}{RT}}$$

$$K_c = \frac{K_f}{c} \Rightarrow \boxed{K_f = K_c \cdot c}$$

$$K_f = \frac{K_c}{c} \Rightarrow \boxed{K_f = K_c \cdot c}$$

$$K_f = K_c \cdot c$$

$$C = \frac{\rho}{M_A}$$

* When A is diffusing and B is non-diff., we get

$$\frac{D_{AB} \cdot C}{l} \ln \frac{c - CA_1}{c - CA_2}$$

$$\frac{D_{AB} \cdot C}{l} \ln \frac{(CA_1 - CA_2)}{CA_1}$$

$$MT C$$

Convective MTC

- Theories
- Simplified
- Plenty of assumptions
- Limited cases

Correlations

- Experimental:
 - using heat/heat transfer analogy

- using analogies:
 - dimensionless constants
- Film Theory
- Penetration theory
- Surface renewal theory
- Boundary layer theory

$$Sh \sim \alpha \sim Nu$$

Shwood no.

$$Sh = Sc = Pr$$

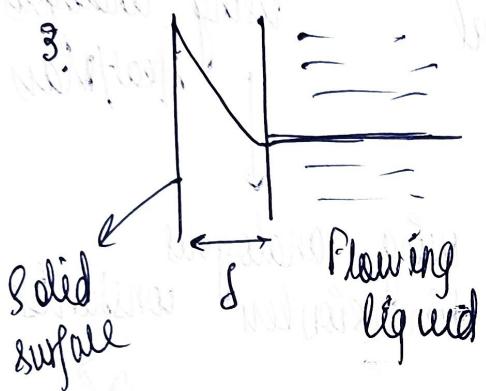
Schmidt- Prandtl no.

Nusselt no.

Film Theory

Assumptions

1. Steady state
2. $N_A = -N_B$ ($V=0 \rightarrow \text{dil.}$)



It says all mass transfer occurs b/w S and w .
try to find the mathematical relⁿ

By Fick's second law,

$$\frac{d^2 C_A}{dz^2} = 0$$

$$BL \rightarrow z=0, C_A = C_{Ai}$$

$$z=\delta, C_A = C_{Ab}$$

Linear

Integrating,

$$C_A = C_{Ai} - (C_{Ai} - C_{Ab}) \frac{z}{\delta}$$

- The mass transfer flux is constant at steady state and is given by

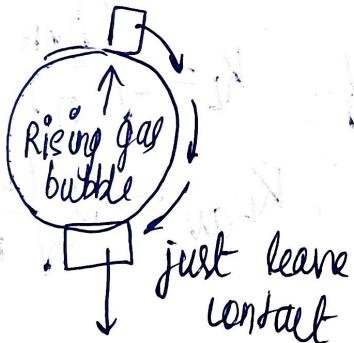
$$N_A = -D_{AB} \frac{dC_A}{dx} = \frac{D_{AB}}{\delta} (C_{Ai} - C_{Ab})$$

$\Rightarrow K_L = \frac{D_{AB}}{S} \rightarrow$ We use K_L for liquid phase

\therefore Mass Transfer Resistance = $\frac{1}{\text{Mass Transfer Coefficient}}$

- * If $V \uparrow, S \uparrow \Rightarrow K_L \downarrow$
- * Mass Transfer Resistance resides only within S .

Penetration Theory



Read the assumptions

$$\star t_c = \frac{d_b}{\bar{U}_b}$$

$$\underline{\text{FC}} \rightarrow t_c, z \geq 0, C_A = C_{Ab}$$

$$\underline{\text{BC}} \rightarrow z = 0; C_A = C_{Ai}$$

$$z = \infty, C_A = C_{Ab}$$

$$-\frac{\partial C_A}{\partial t} = D_{AB} \frac{\partial^2 C_A}{\partial x^2}$$

$$\text{Solve} \rightarrow \frac{C_A - C_{Ab}}{C_{Ai} - C_{Ab}} = 1 - \operatorname{erf}(\eta)$$

$$\text{Where } \eta = \frac{z}{2\sqrt{D_{AB} \cdot t}}$$

* $N_A(t) = -D_{AB} \left[\frac{\partial C_A}{\partial z} \right]_{z=0}$

$$= \sqrt{\frac{D_{AB}}{\pi t}} (C_i - C_{Ab})$$

$$N_A \text{ av} = \frac{1}{t_c} \int_0^{t_c} N_A(t) dt$$

$$= 2 \sqrt{\frac{D_{AB}}{\pi t_c}} (C_{A_i}^0 - C_{Ab})$$

* Instantaneous mass transfer coeff. $K_L = \sqrt{\frac{D_{AB}}{\pi t}}$
 Average " $K_{L \text{ av}} = 2 \sqrt{\frac{D_{AB}}{\pi t_c}}$

Surface Renewal Theory

$$K_L = \sqrt{D_{AB} \cdot S}$$

- S is the fraction of surface area renewed in unit time.

- Increasing turbulence, $\rightarrow MTC \uparrow$

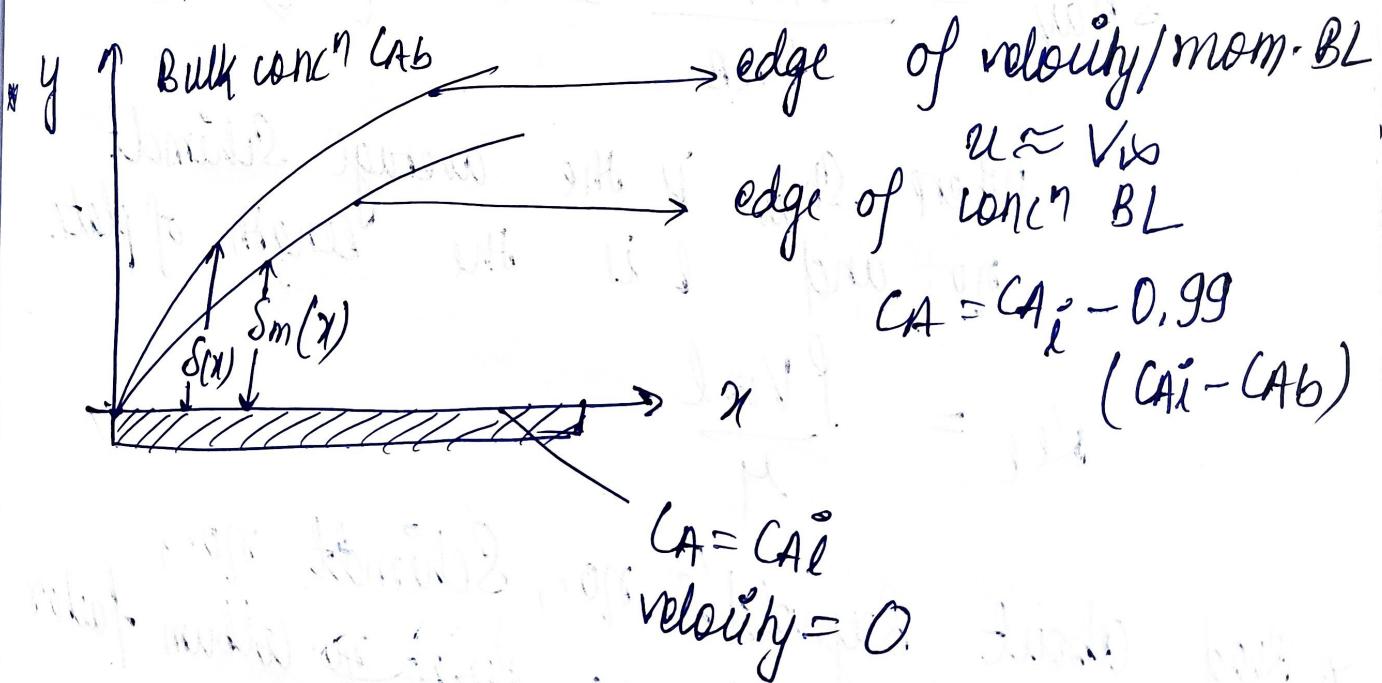
- It is based on the theory that the age of diff. liquid droplets

Bound Layer Theory

The characteristics of the boundary layer depends on the Reynold's no.

$$Re_x = \frac{\rho V_\infty x}{\mu}$$

- Boundary layer flow remains laminar if it is less than 3×10^5 \rightarrow critical Reynold's no.
- If plate is coated with a soluble substance and liquid/gas flows over it, two boundary layers are formed — the velocity BL and the conc' or mass BL.



- The relative thicknesses of the velocity and conc' BL depend on the value of Schmidt no. (Sc)

$$\boxed{\frac{\delta}{\delta_m} = (Sc)^{1/3}}$$

$$Sh_x = \frac{k_{L,n} \cdot x}{D_{AB}} = 0.332 (Re_x)^{1/2} (Sc)^{1/3}$$

Sh_x is the local Sherwood no. and x is the distance of a point from the leading edge of the plate, $k_{L,n}$ is the local mass transfer coefficient & Re_x is

$$Sh_{av} = \frac{k_{L,n} \cdot l}{D_{AB}} = 0.664 (Re_l)^{1/2} (Sc)^{1/3}$$

where Sh_{av} is the average Schmidt no. and l is the length of plate

$$Re_l = \frac{\rho V_{\infty} l}{\mu}$$

* Read about Reynold's no., Schmidt no., Sherwood no., Stanton no., ~~Peclet~~ no., Colburn factor

* Read & Pdf - 98, Correlation for the convective mass transfer coefficient.

Reynold's Analogy

$$St_H = \frac{Nu}{Re Pr} = \frac{f}{2} \rightarrow \text{Stanton no. for Heat transfer}$$

$$St_M = \frac{Sh}{Re Sc} = \frac{f}{2} \rightarrow \text{Stanton no. for mass transfer}$$

f is the friction factor for fluid flowing through pipe.

Prandtl Analogy

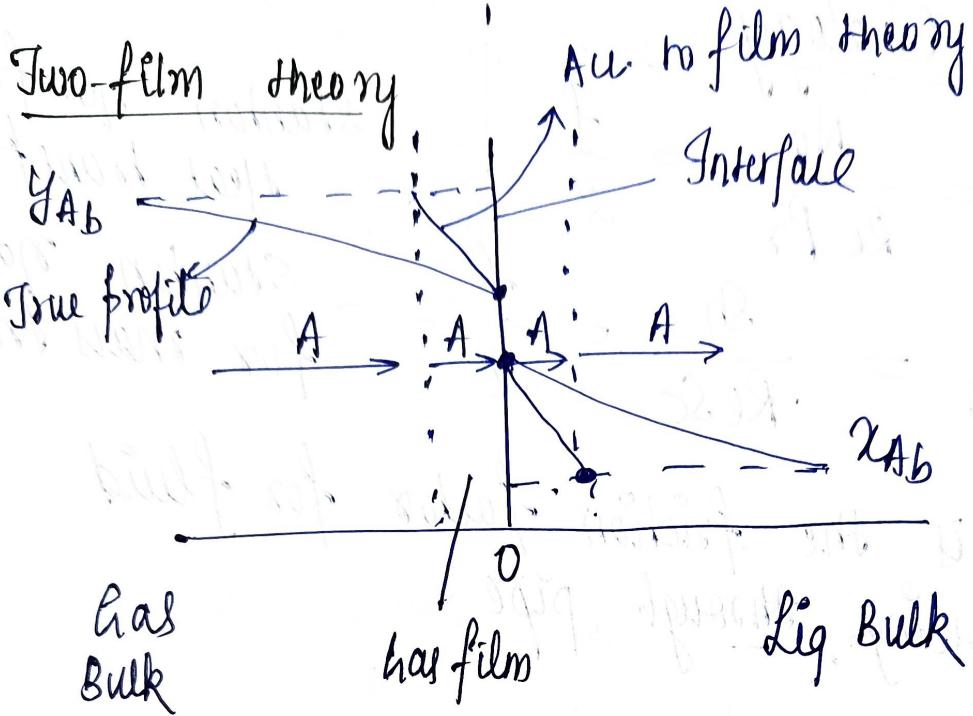
$$St_M = \frac{f/2}{1 + 5\sqrt{f/2(Sc-1)}} , St_H = \frac{f/2}{1 + 5\sqrt{f/2(Pr-1)}}$$

- Prandtl Analogy reduces to Reynold's Analogy if $Pr=1$ and $Sc=1$.

Colburn Analogy

$$\bar{j}_M = St_M Sc^{2/3} = \frac{Sh}{Re Sc^{1/3}} = 0.023 Re^{-0.2}$$

Inter-Phase Diffusion

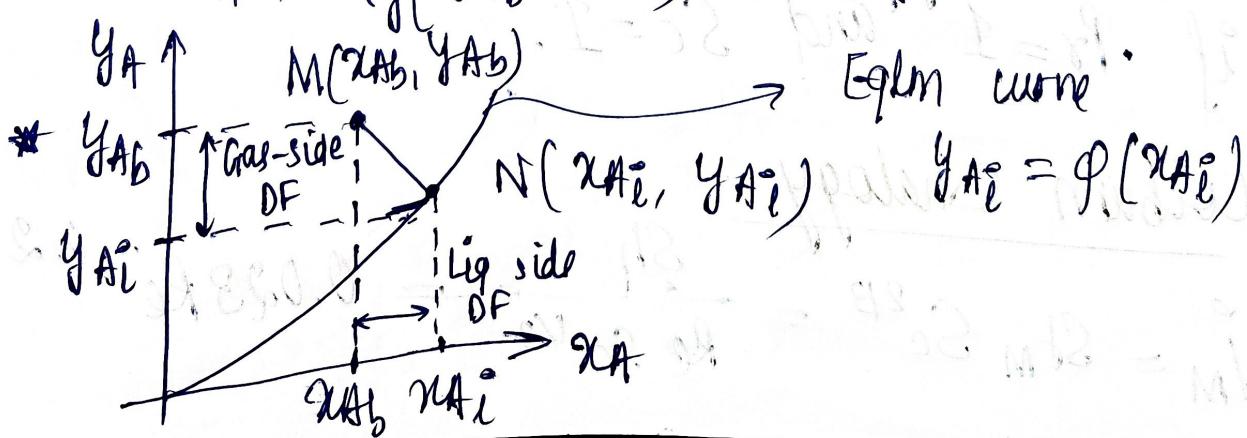


- * y_{Ai} and x_{Ai} are called "interfacial concentrations".

$$y_{Ai} = \phi(x_{Ai}) \text{ At eqm}$$

This is called the "eqm rel"

$$N_A = R_y(y_{Ab} - y_{Ai}) = R_e(x_{Ai} - x_{Ab})$$



$$\frac{y_{Ab} - y_{Ai}^*}{x_{Ab} - x_{Ai}^*} = - \cdot \frac{k_x}{k_y} \quad (\text{line MN})$$

Overall Mass Transfer Coefficient

- Generally, y_{Ai}^* and x_{Ai}^* are very difficult to know, so the previous flux eqn are not used.

Instead, $N_A = k_y (y_{Ab} - y_{Ab}^*)$

$$N_A = k_x (x_{Ab}^* - x_{Ab})$$

where $*$ denotes eqdm condition and k_y and k_x are overall MTC.

$$y_{Ab}^* = \phi(x_{Ab}) \quad \& \quad y_{Ab} = \phi(x_{Ab}^*)$$

* $y_{Ab}^* = \phi(x_{Ab})$ & $y_{Ab} = \phi(x_{Ab}^*)$ overall MTC & k_x is overall liquid phase MTC.

$$N_A = k_y (y_{Ab} - y_{Ai}^*) = k_x (x_{Ai}^* - x_{Ab}) = k_y (y_{Ab} - y_{Ai}^*)$$

$$2) \quad y_{Ab} - y_{Ai}^* = \frac{N_A}{k_y}$$

$$x_{Ai}^* - x_{Ab} = \frac{N_A}{k_x}$$

$$y_{Ab} - y_{Ab}^* = \frac{N_A}{k_y}$$

$$y_{Ab} - y_{Ab}^* = (y_{Ab} - y_{Ai}) + (y_{Ai} - y_{Ab}^*)$$

$$= y_{Ab} - y_{Ai} + \frac{y_{Ai} - y_{Ab}^*}{(x_{Ai} - x_{Ab})} \times ()$$

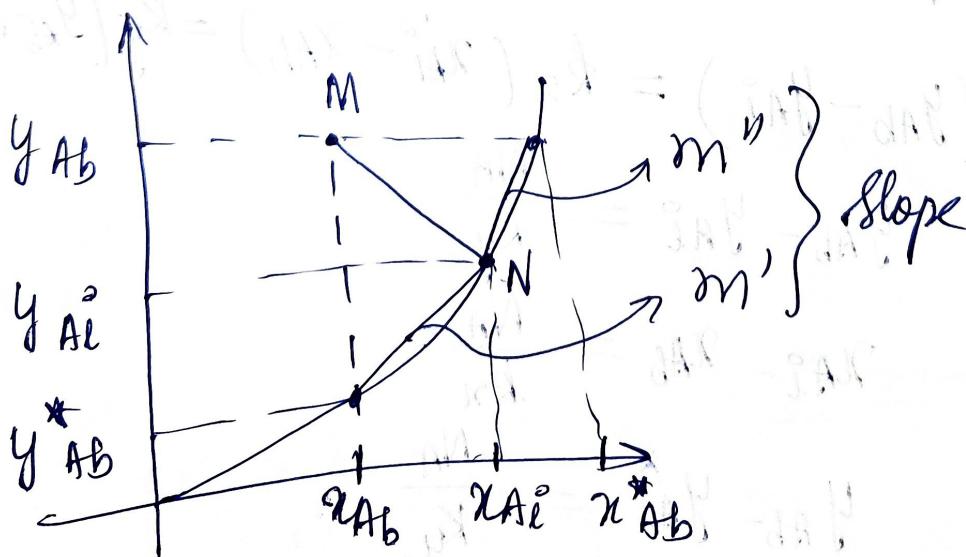
$$\boxed{y_{Ab} - y_{Ab}^* = (y_{Ab} - y_{Ai}) + m'(x_{Ai} - x_{Ab})}$$

$$\Rightarrow \frac{N_A}{K_y} = \frac{N_A}{K_y} + \frac{N_A}{K_x} \cdot m'$$

$$\Rightarrow \boxed{\frac{1}{K_y} = \frac{1}{K_y} + \frac{m'}{K_x}}$$

Similarly,

$$\boxed{\frac{1}{K_x} = \frac{1}{K_x} + \frac{m''}{m' K_y}}$$



- * $\frac{1}{K_y} = \text{individual gas-phase mass transfer}$
- $\frac{m'}{k_x} = \text{individual liquid phase mass transfer}$
(on gas phase basis)
- $\frac{1}{k_x} = \text{individual liquid-phase mass transfer}$
- $\frac{1}{m' k_x} = \text{individual gas-phase mass transfer}$
resistance (on liquid phase basis)

* Fractional resistance offered by gas-phase
 $= \frac{\text{resistance offered by the gas phase}}{\text{total resistance of two phases}}$

$$= \frac{1/k_y}{1/K_y}$$

Fractional mass transfer offered by liquid phase = $\frac{\text{resistance offered by lig phase}}{\text{total resistance of 2 phases}}$

$$= \frac{m'/k_x}{1/K_y}$$