



ملخصات مدار



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انتقال المادة



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* Molecular transport process of (Momentum, heat, mass) $\Rightarrow$ $\text{Rate of transfer} = \frac{\text{driving force}}{\text{resistance}}$

* different conc. $\Rightarrow$ transport transfer from phase to phase or same phase $\Rightarrow$ Mass transfer.
 (region of high conc. $\rightarrow$ lower conc.) $\Rightarrow$ direction of decreasing conc.
 May occur in gas mixture or liquid solution or solid

Fick's law
(Diffusion)

$\Rightarrow$ Flux $\frac{N}{A} = -D \frac{dc}{dx}$ $\rightarrow$ gradient : concentration

* Mass transfer (fluid mixture or across phase boundary) $\Rightarrow$ play major role in industrial process

$\Downarrow$ examples

① Dispersion of gases from stacks.

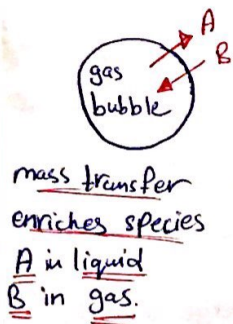
② Distillation columns in petroleum refinery

③ Removal Pollutants from plant discharge streams by absorption in example absorption of CO_2 by water

④ stripping of gases from waste water.

⑤ Adsorption of liquid or gas to solid surface.

⑥ Neutron diffusion within nuclear reactors



reactants or product diffuse in or out of porous catalysts pellets

exchange btw gas and liquid around trays

gas-liquid interface

liquid-solid interface.

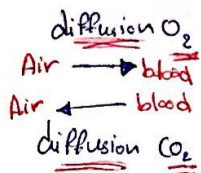
control rod

made of material usually Boron or cadmium

absorb excess neutrons

$\Rightarrow$ by controlling the number of neutrons

$\Rightarrow$ control the rate of fissions



exchange btw lungs and blood capillaries

⑦ Breathing

No Net movement at equilibrium

* examples of mass transfer process $\Rightarrow$ ① Diffusion $\rightarrow$ lump of sugar in coffee $\rightarrow$ make concentration uniform
 ② water evaporate $\rightarrow$ increase humidity or of passing air steam $\rightarrow$ separate solid substance that has dissolved in water
 ③ wood, perfumes

* mass transfer operations are characterized by transfer of substance through another on molecular scale.

* 3 ways to Mass transfer occurs :

① Diffusion ② Advection ③ convection.

- Diffusion : net transport of substances in

↓

① caused by random molecular motion. (Molecular diffusion) or (random walk process)

② take place in mixtures (≥ 2 components)

but heat, momentum need one conformal phases

① Stationary solid
② stagnant fluids
③ Fluids moving in laminar flow
may present in highly developed turbulent flow but near solid surface. (viscous sublayer)

⇒ due to concentration gradient

* in Molecular diffusion with time at the end you achieve uniform conc..

*
$$\text{Flux} = \frac{(\text{mass or moles of species})}{(\text{cross sectional Area}) (\text{time})} \Rightarrow \text{Unit} : \frac{\text{Kg/moles}}{\text{m}^2 \cdot \text{s}}$$

* flux defined with Reference to coordinates

① Fixed in space
② moving with mass average velocity
③ moving with molar $\leq \leq$

* Fick's law for Molecular Diffusion :

$$J_{Az}^* = - C_T D_{AB} \frac{dx_A}{dz} \Rightarrow \text{For : isothermal, isobaric, binary mixture of A, B in stagnant media or laminar flow}$$

J_A^* : molar flux, z direction, molar Avg. velocity coordinates $\Rightarrow$ Unit : $\frac{\text{Kmol of A}}{\text{m}^2 \cdot \text{s}}$

D_{AB} : molecular diffusivity of Molecule A in B $\Rightarrow \frac{\text{m}^2}{\text{s}}$

C_T : total concentration $\Rightarrow \frac{\text{Kmol of (A+B)}}{\text{m}^3}$

z : distance of diffusion $\Rightarrow \text{m}$

x_A : mole fraction of A in mixture of A and B



$$* J_{Az}^* = \frac{\bar{J}_{Az}}{A_m}$$

$$\bar{J}_{Az}: \text{rate of molecular diffusion} \Rightarrow \frac{\text{Kmol of A}}{\delta}$$

$$A_m: \text{mass transfer Area which is normal to transfer direction} \Rightarrow m^2$$

* negative sign $\Rightarrow$ diffusion occurs in the direction of drop in conc.

* mass transfer rate proportional to area $\Rightarrow$ rate can expressed as flux

* Net transfer stops when $\Rightarrow$ conc. uniform

* Fick's law $\Rightarrow$ flux due diffusion (J_{Az}) but not due bulk flow (N_{Az})

$$* C_A = C_T X_A \xrightarrow[\text{if } C \text{ constant}]{} c dx_A = d(CX_A) = dC_A$$

$$\Rightarrow J_{Az}^* = -D_{AB} \frac{dC_A}{dz}$$

$$* C = \frac{P}{RT} = \frac{n}{V}$$

$$* J_{Az}^* = \frac{D_{AB} (P_{A1} - P_{A2})}{RT (z_2 - z_1)} \Rightarrow \text{steady state, constant total pressure}$$

$$* \text{Equimolar Counter diffusion} \Rightarrow J_{Az}^* = -J_{Bz}^*$$

$$P = P_A + P_B = \text{constant} \Rightarrow C = C_A + C_B = \text{constant}$$

$$D_{AB} = D_{BA} \quad \leftarrow \quad dC_A = -dC_B$$

$$* P_B = P - P_A$$

$$* R = 8814.8 \frac{m^3 \cdot Pa}{kg \cdot mol \cdot K} = 82.057 \frac{cm^3 \cdot atm}{g \cdot mol \cdot K}$$



* Advection: ① net transport of substances by the moving fluid

② not include transport by diffusion

③ can't happen in solid.

* Convection: net transport caused by both $\begin{cases} \text{advection} \\ \text{diffusive} \end{cases}$

↓ depends on

① transport prop.

② dynamic charc. of moving fluid.

$$N_{AZ} = K_c \Delta C_A$$

↓ molar mass transfer ↓ convective mass transfer coefficient

similar to Newton law of cooling.

* Summary slide 40 important.

* General flux equation $\Rightarrow$

$$\text{total mass transported} = \text{mass transport by diffusion} + \text{mass transport by bulk fluid}$$

Stefan and Maxwell using Kinetic theory.

$$\begin{aligned} V_{A, \text{diffusion}} \text{ (m/s)} &= \frac{J_A^* \text{ (mol/m}^2\text{.s)}}{C_A \text{ (mol/m}^3\text{)}} \\ V_{\text{bulk, avg}} &= \frac{\sum_{i=1}^n C_i V_i}{C} \end{aligned} \Rightarrow V_i \text{ (total)} = V_{\text{bulk}} + V_{\text{diff}}$$

$$* N_A = C_A V_A$$

$$* N_B = C_B V_B$$

$$V_{\text{bulk}} = \frac{(N_A + N_B)}{\frac{C}{T}}$$

$$N_i = \frac{W_i \text{ (mol/s)}}{A \text{ (m}^2\text{)}}$$

total molar flux by convection.

$$\Rightarrow N_A = \underbrace{-D_{AB} \frac{dc_A}{dz}}_{\text{diffusion}} + \underbrace{\frac{C_A}{C_T} (N_A + N_B)}_{\text{Bulk flow}}$$

general flux equation

Note: if C_A too small (mixture dilute in A), bulk flow term ignored $\Rightarrow N_A = -D_{AB} \frac{dc_A}{dz}$

$$* N_A = - \frac{D_{AB}}{RT} \frac{dP_A}{dz} + \frac{P_A}{P} (N_A + N_B)$$

$$* C_A = \frac{n_A}{V} = \frac{P_A}{RT} \rightarrow \text{Partial pressure.}$$

$$* C_T = \frac{n_T}{V} = \frac{P}{RT}$$

$$* N_A = - C_T D_{AB} \frac{dx_A}{dz} + x_A (N_A + N_B)$$

$$* x_A = \frac{P_A}{P} = \frac{N_A}{N_A + N_B} = \frac{C_A}{C_T}$$

* Diffusivity $\Rightarrow$

$$* D_{AB} = - \frac{J_{A2}}{dc_A/dz} = \left(\frac{m^2}{s} \right) \rightarrow L^2$$

* gases at low density: $D_{AB} \uparrow$ with Temp

$D_{AB} \downarrow$ with Pressure
indp. with composition

depends on: Pressure, Temp., composition

* liquid and solids: $D_{AB} \uparrow$ with Temp.

depend with composition

* Diffusivity in gases:

$$D_{AB}(T_2, P_2) = D_{AB}(T_1, P_1) \left(\frac{P_1}{P_2} \right) \left(\frac{T_2}{T_1} \right)^{3/2}$$

Hirschfelder extrapolation $\Rightarrow * D_{AB} \propto \frac{1}{P}, D_{AB} \propto T^{3/2}$
(below 25 atm).

$$D_{1\text{-mixture}} = \frac{1}{\frac{x_2'}{D_{1-2}} + \frac{x_3'}{D_{1-3}} + \dots + \frac{x_n'}{D_{1-n}}}$$

$$x_n' = \frac{x_2}{x_2 + x_3 + \dots + x_n}$$

$$D_{AB} = 10^{-3} T^{1.75} \left[\frac{1}{M_A} + \frac{1}{M_B} \right]^{1/2}$$

$$P \left[(\sum V_A)^{1/3} + (\sum V_B)^{1/3} \right]^2$$

Fuller method.

Diff. for binary system.

$$* D_{AB} \propto \frac{1}{P}, D_{AB} \propto T^{1.75}$$

D_{AB} : in cm^2/s

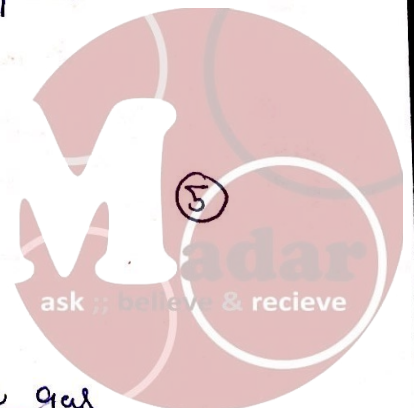
P : in atm

M : molecular weight

T : in K

V : volume diffusion (الجلد)

* Diff. in liquid ten thousand time slower than dilute gas



* Diff. in liquid $\Rightarrow$ nearer to $10^{-5} \text{ cm}^2/\text{s}$.

$$D_{AB} = \frac{9.96 \times 10^{-12} T}{\mu V_A^{1/3}} \quad \text{K}$$

viscosity of solution (Kg/ms) μ
 Solute Molar volume at Normal boiling point (m³/Kmol) V_A (دولت درجہ)

very large spherical dilute solute A of 1000 M. weight or greater diffusing in liq. solvent B of small molecules

$\Rightarrow$ Proportional to $\frac{1}{\mu}$ and T

$$\left(\frac{D_{AB} \mu}{T} \right)_{T_2} = \left(\frac{D_{AB} \mu}{T} \right)_{T_1}$$

$$D_{AB} = \frac{7.4 \times 10^{-8} (\phi M_B)^{1/2} T}{\mu_B V_A^{0.6}} \quad \text{K}$$

parameter for solvent ϕ
 M. weight M_B
 viscosity of B in cp μ_B

Smaller molecules A diff. in dilute liq. solution of solvent B

$\Rightarrow$ Proportional to $\frac{1}{\mu_B}$ and T

* if V_A not available in Tables $\Rightarrow$ Tyn and chus correlation.

$$V_A = 0.285 V_c^{1.048}$$

critical volume of solute A (cm³/g mol)

$$D_{AB}^0 = \frac{8.928 \times 10^{-10} T (1/n_+ + 1/n_-)}{(1 + \lambda_+ + 1/\lambda_-)} \quad \text{K}$$

298.2 (25°C)
 valence of cation n_+
 valence anion n_-
 limiting ionic conductance in very dilute solution. λ_+
 limiting ionic conductance in very dilute solution. λ_-

Electrolytes in liquid (dilute liquid) of solvent B

$\Rightarrow$ Proportional to T

* Diff. in solids $\Rightarrow$ btw $5 \times 10^{-14} - 1 \times 10^{-10}$

$\Rightarrow$ less than liquid, liquid less than gas

$\Rightarrow$ important in catalysis.



* $\frac{\partial N_{A2}}{\partial z} + \frac{\partial C_A}{\partial t} = 0 \xrightarrow[\text{state}]{\text{steady}}$ $\frac{\partial N_{A2}}{\partial z} = 0 \Rightarrow \underline{N_{A2} = \text{constant}}$

1D, no chemical Rxn.

$N_A = -C_T D_{AB} \frac{dx_A}{dz} + x_A (N_A + N_B) \Rightarrow \underline{\text{general flux equation}}$

$\Rightarrow \text{after Integrate } N_A = \frac{N_A}{(N_A + N_B)} \frac{C_T D_{AB}}{z} \ln \left(\frac{\frac{N_A}{N_A + N_B} - \frac{C_{A2}}{C_T}}{\frac{N_A}{N_A + N_B} - \frac{C_{A1}}{C_T}} \right) \Rightarrow \underline{\text{difficult to find by solving in trial and error}}$

Cases to simplify it

① Diffusing of A through stagnant, non-diffusing B:

$\Downarrow$
B is moving but not diffusing
in the path.

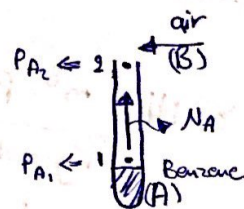
impermeable to component B $\Rightarrow$ can't pass through $\Rightarrow \underline{N_B = 0}$

* Evaporation of pure liquid A (benzene), large amount of air passed over the top(B)

A diffuse through B

B insoluble in A $\Rightarrow$ B can't diffuse $\Rightarrow \underline{N_B = 0}$

at point 2 $\Rightarrow \underline{P_{A2} = 0}$ (large volume of air is passing through)



* NH₃ vapor(A), Air(B) by water.

air $\Rightarrow$ source & no sink $\Rightarrow$ not soluble in water $\Rightarrow$ not diffusing $\rightarrow \underline{N_B = 0}$

NH₃ $\Rightarrow$ source, sink

* $N_A = -C_T D_{AB} \frac{dx_A}{1-x_A} \frac{dz}{dz} \xrightarrow{\text{Integrate}}$

$N_A = \frac{C_T D_{AB}}{z_2 - z_1} \ln \left(\frac{1 - x_{A2}}{1 - x_{A1}} \right)$
 $= \frac{C_T D_{AB}}{z_2 - z_1} \ln \left(\frac{C_T - C_{A2}}{C_T - C_{A1}} \right)$

$x_A = 1 - (1 - x_{A1}) \exp \left(\frac{N_A (z - z_1)}{C_T D_{AB}} \right)$

$x_A = \frac{C_A}{C_T}$

$P_A = C_A RT$

$P = C_T RT$

$x = \frac{P_A}{P}$

$$(*) N_A = \frac{P D_{AB}}{RT(z_2 - z_1)} \ln \left(\frac{P - P_{A2}}{P - P_{A1}} \right)$$

$$(*) N_A = \frac{C_T D_{AB}}{z_2 - z_1} \frac{(x_{A1} - x_{A2})}{x_{B,lm}}$$

$$N_A = \frac{P D_{AB}}{RT(z_2 - z_1)} \frac{(P_{A1} - P_{A2})}{P_{B,lm}}$$

$$(*) C_A \text{ low, diluted} \Rightarrow \begin{cases} x_{B,lm} = 1 \\ P_{B,lm} = P \end{cases}$$

$$x_B = 1 - x_A \Rightarrow$$

$$(*) x_{B,lm} = \frac{x_{A1} - x_{A2}}{\ln \left(\frac{1 - x_{A2}}{1 - x_{A1}} \right)} = \frac{x_{B2} - x_{B1}}{\ln \left(\frac{x_{B2}}{x_{B1}} \right)}$$

$$P_B = P - P_A \Rightarrow$$

$$(*) P_{B,lm} = \frac{P_{B2} - P_{B1}}{\ln \left(\frac{P_{B2}}{P_{B1}} \right)} = \frac{(P - P_{A2}) - (P - P_{A1})}{\ln \left(\frac{P - P_{A2}}{P - P_{A1}} \right)}$$

N_A depend on driving force, distance.

$$(*) 1 \text{ atm} = 1.01325 \times 10^5 \text{ Pa.}$$

$$(*) D_{AB} \text{ from } m^2/s \rightarrow ft^2/h \Rightarrow \text{conversion} = 3.875 \times 10^{-4}$$

$$(*) R = 8314 \frac{m^3 \cdot Pa}{kg \cdot mol \cdot K}$$

$$= 82.057 \frac{cm^3 \cdot atm}{g \cdot mol \cdot K}$$

$$= 0.7302 \frac{ft^3 \cdot atm}{lb \cdot mol}$$

(8)

Note: ① N_A constant mean flux along diffusion path constant.
but conc. is different.

② $-r_A$ term $\Rightarrow$ Rxn within Diffusion path & Homogeneous.

② Equimolar Counter Diffusion :

$$* N_A = -N_B$$

$$N_A = -D_{AB} \frac{dC_A}{dz} + X_A (N_A + N_B)$$

$$\Rightarrow N_A = -D_{AB} \frac{dc_A}{dz} \xrightarrow{\text{Integrate}} N_A = \frac{D_{AB}}{z_2 - z_1} (C_{A_1} - C_{A_2})$$

$$\downarrow \quad \star C_A = \frac{n_A}{V} = \frac{P_A}{RT}$$

$$N_A = \frac{D_{AB}}{RT(z_2 - z_1)} (P_{A_1} - P_{A_2})$$

* Conc. A at any location
along diffusion path

$$\Rightarrow N_A = \frac{D_{AB}}{(z_2 - z_1)RT} (P_{A_1} - P_{A_2})$$

$$N_A = \frac{D_{AB}}{(z'_1 - z_1)RT} (P_{A_1} - P_{z'_1})$$

Equating
 $\Rightarrow P_{z'_1} = P_{A_2}$

or

$$\textcircled{2} \frac{C_A - C_{A_1}}{C_{A_1} - C_{A_2}} = \frac{z - z_1}{z_1 - z_2}$$

③ Relation b/w N_A & N_B fixed by reaction stoichiometry



$$\frac{N_A}{m} = -\frac{N_B}{n} \Rightarrow N_B = -\left(\frac{n}{m}\right) N_A$$

$N_B = - \left(\frac{\lambda_A}{\lambda_B} \right) N_A$

by latent heat of vaporization → more volatile comp. transfer from liq → vap
less s s s s vap → liq.

ask : believe & recieve

9

* Pseudo steady state diffusion $\Rightarrow$ length diff. path changes a small amount over a long period. time.

$\Downarrow$

molar flux
stagnant

$$N_A = \frac{C_T D_{AB}}{z} \frac{(x_{A1} - x_{A2})}{x_{B,lm}}$$

$z_2 - z_1$ (length path)

$$\textcircled{2} N_A A = \frac{dN}{dt} = \frac{\text{mass}}{M.W} \rightarrow \rho \rightarrow A_2$$

$$\Rightarrow N_A = - \frac{\rho}{M_A} \frac{dz}{dt}$$

$$\Rightarrow \frac{\rho_{A, L}}{M_A} \frac{dz}{dt} = \frac{C_T D_{AB}}{z} \frac{(x_{A1} - x_{A2})}{x_{B,lm}}$$

Molar density

$$t = \frac{\rho_{A, L} x_{B,lm} / M_A}{C_T D_{AB} (x_{A1} - x_{A2})} \left[\frac{z_t^2 - z_0^2}{2} \right]$$

$$D_{AB} = \frac{\rho_{A, L} x_{B,lm}}{M_A C_T (x_{A1} - x_{A2})} \left[\frac{z_t^2 - z_0^2}{2} \right]$$

* Diffusion into infinite stagnant Media $\Rightarrow$ large media ($N_B = 0$) W_A constant, N_A not constant because r changes.

$$N_A = - \frac{C_T D_{AB}}{1 - x_A} \frac{dx_A}{dr}$$

$$A = 4\pi r^2$$

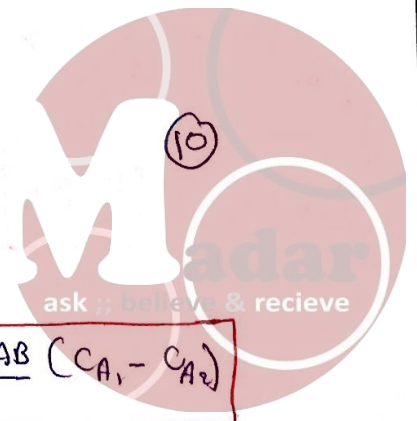
$$W_A = 4\pi r^2 N_A = 4\pi r_0^2 N_{A0}$$

$$C_T = \frac{P}{RT}$$

$$C_A = \frac{P_{A1}}{RT}$$

$$W_A = \frac{4\pi C_T D_{AB}}{1/r_0} \ln \left(\frac{1 - x_{A2}}{1 - x_{A1}} \right)$$

$$N_{A0} = \frac{D_{AB} P}{RT r_0} \frac{(P_{A1} - P_{A2})}{P_{B,lm}} \xrightarrow{\frac{P_{B,lm} = P}{P_{A1} \text{ small}}} N_{A0} = \frac{2 D_{AB}}{r_0} (C_{A1} - C_{A2})$$



$$t = \frac{P_A}{M_A} \frac{1}{2 C_T D_{AB}} \frac{(r_i^2 - r_f^2)}{\ln \left(\frac{1-x_{A2}}{1-x_{A1}} \right)}$$

$$= \frac{P_A R T (r_i^2 - r_f^2)}{2 M_A D_{AB} P} \frac{P_{B,lm}}{(P_{A1} - P_{A2})}$$

* Diffusion through varying Area $\Rightarrow$

$$N_A = - \frac{C_T D_{AB}}{1-x_A} \frac{dx_A}{dz}$$

$$N_A = \frac{-D_{AB}}{RT \left(\frac{1-P_A}{P} \right)} \frac{dP_A}{dz}$$

(11)

$$r = \left(\frac{(r_2 - r_1)}{(z_2 - z_1)} \right) z + r_1$$

$$\bar{N}_A = \frac{\pi D_{AB} P}{RT} \frac{r_1}{z} \left[r_1 - (r_1 - r_2) \left(\frac{z}{L} \right) \right] \ln \frac{P}{P - P_A^v}$$

* Diffusion in liquid $\Rightarrow$

$$N_A = \frac{D_{AB}}{z_2 - z_1} (C_{A1} - C_{A2}) = \frac{C_{av} D_{AB}}{z_2 - z_1} (x_{A1} - x_{A2})$$

$$C_{av} = \frac{\frac{P_1}{M_1} + \frac{P_2}{M_2}}{2}$$

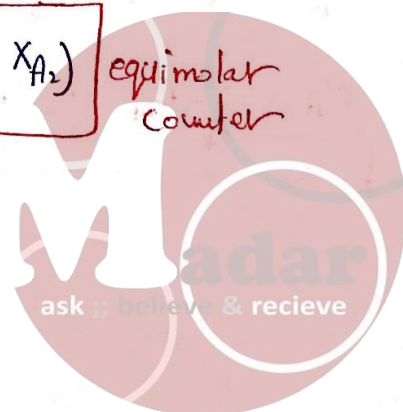
$$\Rightarrow N_A = \frac{D_{AB}}{z} \left(\frac{P}{M} \right)_{av} (x_{A1} - x_{A2})$$

equimolar counter

$$N_A = \frac{D_{AB}}{(z_2 - z_1) X_{Bm}} \left(\frac{P}{M} \right)_{av} (x_{A1} - x_{A2})$$

not diffusing B

$$X_{Bm} = \frac{x_{A1} - x_{A2}}{\ln(1-x_{A2}/1-x_{A1})}$$



* Diffusivity in solids $\Rightarrow$

- following Fick's law

$$N_A = D_{AB} \frac{C_{A1} - C_{A2}}{z_2 - z_1} \quad \text{planar surface.}$$

$$W_A = 2\pi L D_A \frac{(C_{Ai} - C_{Ao})}{\ln\left(\frac{r_o}{r_i}\right)}$$

$$C_A(r) = C_{Ai} - \frac{(C_{Ai} - C_{Ao})}{\ln\left(\frac{r_o}{r_i}\right)} \ln\left(\frac{r}{r_i}\right)$$

$$N_A = \frac{W_A}{2\pi r L}$$

cylindrical
surface

Note: W_A constant

$$W_A = 4\pi r_i r_o D_A \frac{(C_{Ai} - C_{Ao})}{r_o - r_i}$$

$$N_A = \frac{W_A}{4\pi r^2}$$

spherical
surface

- following Nature of solid: type, size of pores.

2019/08/10
15 (slides)

① Liquid in solids

$$D_{Aef} = (\varepsilon / K_t^2) D_{AB}$$

$$N_A = \frac{\varepsilon}{K_t^2} D_{AB} \frac{C_{A1} - C_{A2}}{z_2 - z_1}$$

ε : volume void fraction

K_t : tortuosity factor



②

* Diff. Gases in Solid: diameter Pores, mean free path, size of pores.

$$\lambda_A = \frac{3.2 M_A}{P} \left[\frac{RT}{2\pi M_A} \right]^{0.5} \Rightarrow K_n = \frac{\lambda}{d_{\text{pore}}} \quad \text{Knudsen number}$$

mean free path

λ : m
 T : K
 M : kg/m.s

P : N/m²
 R : 8314 J/Kmol.K

$\Rightarrow K_n < 0.01$: indp. of nature of solid

$$N_A = - \frac{D_{AB} P}{RT} \frac{dy_A}{dz} + y_A (N_A + N_B)$$

$\Rightarrow K_n > 10$

$$D_{KA} = 4850 d_{\text{pore}} \sqrt{\frac{T(K)}{M_A}} \quad \text{Knudsen diffusion}$$

$$N_A = -D_{KA} \frac{dC_A}{dz} = -\frac{D_{KA}}{RT} \frac{dp_A}{dz}$$

$$= \frac{D_{KA} P}{RT \Delta z} (y_{A1} - y_{A2})$$

* Knudsen diffusion significant $\Rightarrow$ low pressure, small diameter

⑬

* $0.1 < K_n < 1 \Rightarrow$ measurable but moderate rate in overall diffusion

$K_n > 1 \Rightarrow$ important

$$0.01 < K_n < 10 \Rightarrow \frac{1}{D_{Ae}} = \frac{1}{D_{AB}} + \frac{1}{D_{KA}}$$

* Pores twisted interconnected $\Rightarrow D'_{Ae} = \epsilon^2 D_{Ae}$

