

CHE 318 L06

Jan - 16 2026

Continue from L05 examples

Example 6.3-2 (Geankoplis)

Diffusion of A NH_3 in B water 278K 4.0 mm thick
at contact with organic liquid

Concentration of NH_3 is constant equilibrium conc

of NH_3 at surface = 2.0 wt% NH_3

$$\rho_{\text{aq}} = 991.7 \text{ kg/m}^3$$

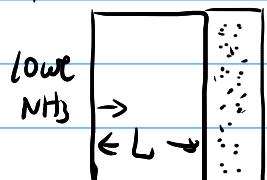
(NH_3 aq) the other end low wt% $P = 961.7 \text{ kg/m}^3$

$$D_{AB} = 1.24 \times 10^{-9} \text{ m}^2/\text{s}$$

A) Calculate S.S N_A in $\text{kg/m}^2/\text{s}$

B) N_B ?

$$\rho_1 = 961.7 \text{ 2.0 wt%}$$



$$L = 4 \text{ mm}$$

We know from Water-organic impermeable
 $\Rightarrow N_B = 0$ stagnant B

$$N_A = \frac{D_{AB} C_{av}}{L} \cdot \frac{1}{x_B m} (x_{A1} - x_{A2})$$

1. weight fraction \rightarrow molar fraction

$$x_A = \frac{\frac{w_A}{M_A}}{\frac{w_A}{M_A} + \frac{w_B}{M_B}}$$

$$\begin{aligned} \tilde{M} &= \frac{[\text{mass}]}{[\text{mole}]} = \frac{m}{\frac{m \cdot w_A}{M_A} + \frac{m \cdot w_B}{M_B}} \\ &= \frac{1}{\frac{w_A}{M_A} + \frac{w_B}{M_B}} \end{aligned}$$

$$x_B = 1 - x_A$$

$$\bar{M}_1 = \frac{1}{\frac{0.10}{17.03} + \frac{0.90}{18.02}} = \frac{1}{0.0558} = 17.92 \text{ kg/kg mol}$$

$$\bar{M}_2 = \frac{1}{\frac{0.02}{17.03} + \frac{0.98}{18.02}} = 17.99 \text{ kg/kg mol}$$

$$Cav = \frac{1}{2} \left(\frac{\rho_1}{M_1} + \frac{\rho_2}{M_2} \right) = 0.5 \times \left(\frac{961.7}{17.92} + \frac{997.1}{17.99} \right) = 54.55 \text{ kg mol/m}^3$$

$$\chi_{A1} = \frac{\frac{0.10}{17.03}}{\frac{0.10}{17.03} + \frac{0.90}{18.02}} = 0.105 \quad \chi_{B1} = 0.895$$

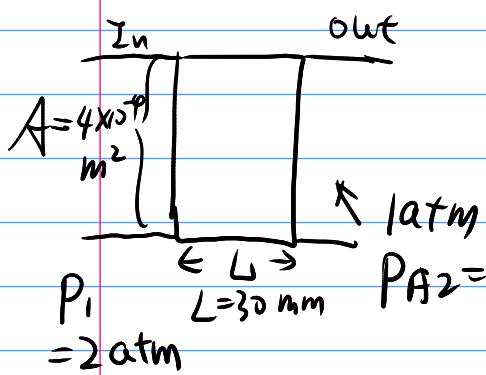
$$\chi_{A2} = \frac{\frac{0.02}{17.03}}{\frac{0.02}{17.03} + \frac{0.98}{18.02}} = 0.0211 \quad \chi_{B1} = 0.979$$

$$\chi_{Bm} = \frac{0.895 - 0.979}{\ln\left(\frac{0.895}{0.979}\right)} = 0.936$$

$$N_A = \frac{1.24 \times 10^{-9} \times 54.55}{0.004} \times \frac{1}{0.936} \times (0.105 - 0.0211)$$

$$= 1.52 \times 10^{-6} \text{ kg mol/m}^2/\text{s}$$

Example 6.5.1 Diffusion through rubber (solubility)



total leakage of CO_2 (amount / s)

$$S = 0.90 \text{ m}^3 \text{ (STP)}$$

$$D = 0.11 \times 10^{-9} \text{ m}^2/\text{s}$$

$$A N_A = \frac{D_{AB} \cdot (C_{A1} - C_{A2})}{Z_{A1} - Z_{A2}} \cdot A \quad C_A = \frac{S P_A}{22.414} \text{ (kg mol/m}^3\text{)}$$

$$= \frac{D_{AB} \cdot S \cdot (P_{A1} - P_{A2})}{(Z_{A1} - Z_{A2}) \cdot 22.414} \cdot A$$

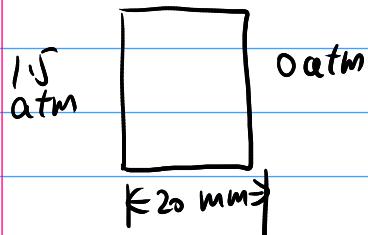
$$= \frac{0.11 \times 10^{-9} \times 0.90 \times (2 - 0)}{0.03 \times 22.414} \cdot 4.0 \times 10^{-4}$$

$$= 1.178 \times 10^{-13} \underbrace{\text{kg mol/s}}$$

amount transferred / time

Example 6.5 - 3

Diffusivity vs permeability



permeability

$$P_M = D_{AB} \cdot S$$

$$D_{AB} = 0.85 \times 10^{-9} \text{ m}^2/\text{s}$$

$$S = 0.040$$

$$P_M = 0.342 \times 10^{-10} \text{ m}^3/(\text{m}^2 \cdot \text{atm}/\text{m})$$

$$\text{a) } D_{AB} = \frac{P_M}{S} = \frac{0.342 \times 10^{-10}}{0.040} = 8.55 \times 10^{-10} \text{ m}^2/\text{s}$$

\hookrightarrow same as D_{AB} table

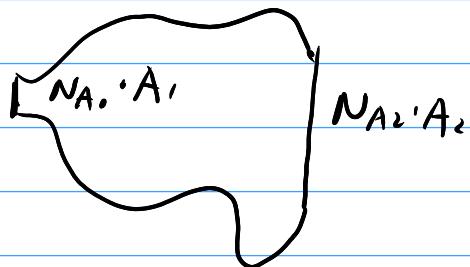
$$\text{b) N}_2 \text{ S.S.}$$

$$N_A = \frac{P_M (P_{A1} - P_{A2})}{22.414 \text{ L}} = \frac{0.342 \times 10^{-10} \cdot (1.5 - 0)}{22.414 \cdot 0.020}$$

$$= 1.144 \times 10^{-10} \text{ kg mol/m}^2/\text{s}$$

Diffusion through varying cross-section areas

Steady State = $\text{In} \cdot \text{Area}_{\text{in}} - \text{Out} \cdot \text{Area}_{\text{out}} = 0$



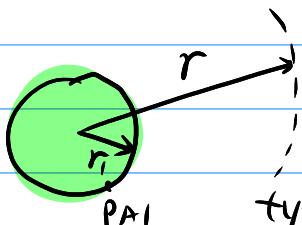
$$N_{A1} \cdot A_1 = N_{A2} \cdot A_2$$

Can be used to solve diffusion through

- ① sphere
- ② cylinder
- ③ tube with varying dia.
- ④ (Any given $A = A(z)$ system)

mole/s $\bar{N}_A = N_A \cdot \bar{A}$ *area*

Case 1: through sphere



Which condition?

- 1) Steady state
- 2) Stagnant B

typical case: evaporation of droplet
| sublimation of solid organic sphere

Governing equation (see Stag B)

Don't use the full solution for 1D! Use the ODE form

$$N_A = - \frac{D_{AB}}{RT} \frac{dP_A}{dr} + \frac{P_A}{P_T} N_A \quad \left(\text{Spherical} \right. \\ \left. \nabla \psi |_r = \frac{\partial \psi}{\partial r} \right)$$

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

$N_A(r)$ is changing \rightarrow Cannot appear in L.H.S
 $\bar{N}_A(r) = N_A \cdot 4\pi r^2$ is constant \rightarrow OK. for L.H.S

$$\frac{\bar{N}_A dr}{4\pi r^2} = - \frac{D_{AB}}{RT} \frac{1}{1 - \frac{P_A}{P_T}} dP_A$$



Integrate

$$\int_{r_1}^{r_2} \frac{\bar{N}_A}{4\pi r^2} dr = - \int_{P_{A1}}^{P_{A2}} \frac{D_{AB}}{RT} \frac{1}{1 - \frac{P_A}{P_T}} dP_A$$

$$\frac{\bar{N}_A}{4\pi} \left(-\frac{1}{r} \right) \Big|_{r_1}^{r_2} = - \frac{D_{AB}}{RT} \cdot P_T \cdot \left[\ln \left(1 - \frac{P_A}{P_T} \right) \right] \Big|_{P_{A1}}^{P_{A2}}$$

$$\frac{\bar{N}_A}{4\pi} \left(\frac{1}{r_1} - \frac{1}{r_2} \right) = \frac{D_{AB} P_T}{RT} \ln \left(\frac{P_T - P_{A2}}{P_T - P_{A1}} \right)$$

Conditions

- 1) P_{A1} : equilibrium pressure / vapor pressure at interface
- P_{A2} : partial pressure at far end
 Could be 0 if $r \rightarrow \infty$

We can simplify this eqn. for some conditions

$$\textcircled{1} \quad r_2 \gg r_1 \quad (r_2 \rightarrow \infty)$$

example droplet evaporating / naphthalene sphere sublimation



Use the ρ_m term, we have

$$\frac{\bar{N}_A}{4\pi} \cdot \frac{1}{r_i} = \frac{D_{AB}}{RT} \frac{P_T}{P_{Bm}} (P_{A1} - P_{A2})$$

$$N_{AI} = \frac{\overline{N_A}}{4\pi r^2} = \frac{D_{AB}}{RT} \frac{P_T}{P_{gm}} (P_{A1} - P_{A2}) \cdot \frac{1}{r}$$

(Do we have the correct unit?)

(looks like diffusion through sphere of radius r_i , has the same flux as through stagnant film with thickness = r_i)

If $p_{A1} \ll p_T \Rightarrow p_{Bm} \approx p_T$

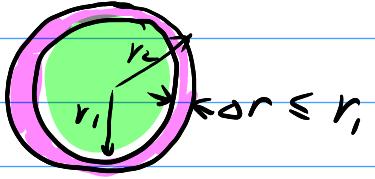
Use CA form ($P_A = \text{CART}$)

$$N_{AI} = \frac{D_{AB}}{r} \cdot (C_{A1} - C_{A2})$$

↳ more used in liquids

② If $\Delta r = r_2 - r_1 \ll r_1$ (thin membrane through sphere)

$$\frac{1}{r_1} - \frac{1}{r_2} = \frac{r_2 - r_1}{r_1 r_2} \approx \frac{\Delta r}{r_1^2}$$



$$\frac{4\pi r_1^2 \cdot N_A}{4\pi} \left(\frac{1}{r_1} - \frac{1}{r_2} \right) = \frac{D_{AB} P_T}{RT} \ln \left(\frac{P_T - P_{A2}}{P_T - P_{A1}} \right)$$

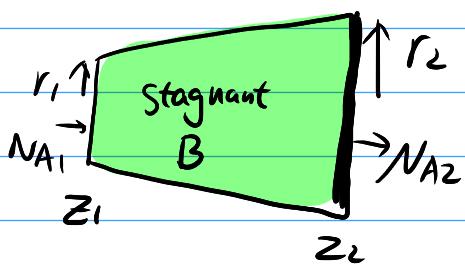
\downarrow
 $\Delta r / r_1^2$

$$\frac{4\pi r_1^2 \cdot N_A}{4\pi} \cdot \frac{\Delta r}{r_1^2} = \frac{D_{AB}}{RT} \frac{P_T}{P_{Bm}} (P_{A1} - P_{A2})$$

$$N_A = \frac{D_{AB}}{RT} \cdot \frac{1}{\Delta r} \cdot \frac{P_T}{P_{Bm}} (P_{A1} - P_{A2})$$

\downarrow
membrane thickness ! just like 1D
Stagnant B solution

Case 2 Diffusion through non-uniform area Conduit

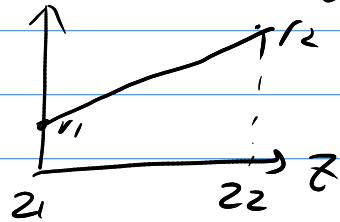


Again, use the ODE form of N_A

$r(z)$ profile: linear

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

$$\frac{\bar{N}_A}{\pi r^2} = - \frac{D_{AB}}{RT} \frac{dp_A}{\left(1 - \frac{P_A}{P_T}\right)}$$

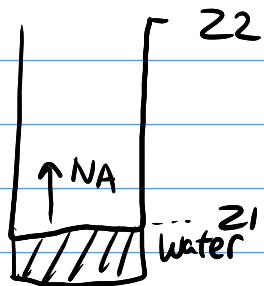


→ Solve

$$\frac{\bar{N}_A}{\pi} \int_{z_1}^{z_2} \frac{dz}{\left[\left(\frac{r_2 - r_1}{z_2 - z_1} \right) z + r_1 \right]^2} = - \frac{D_{AB}}{RT} \int_{P_{A1}}^{P_{A2}} \frac{dp_A}{1 - \frac{P_A}{P}}$$

Can you solve this ?

Example 3 (6.2 - 3) Diffusion with change path length



Water evaporates → level decrease

time of level drop from z_0 to z_f
(t_f)

① Draw scheme

② which condition? Stagnant B

③ Which assumption?

Pseudo steady state \Rightarrow 1) Flux at each t follows Stagnant B
2) $t \rightarrow t + \Delta t$ $z_2 - z_1$ increases

④ Governing eq (using log-mean pressure form)

$$\text{at each } t \quad N_A = \frac{D_{AB}}{RT(z_2 - z_1)} \cdot \frac{P_T}{P_{Bm}} (P_{A1} - P_{A2})$$

$\downarrow \quad \downarrow \quad \uparrow$
 $P_{B1} - P_{B2}$ vapor pressure $= \text{dry air}$
 $\ln \frac{P_{B1}}{P_{B2}}$

Mass balance

$$I_n - O_{\text{out}} + G_{\text{en}} = A_{\text{cc}}$$

$$O - N_A + D = - \frac{(\text{mass loss})}{(\text{time})}$$



$$\int N_A \cdot dt = \frac{\int dz \cdot \rho_A}{M_A} \quad \text{and sur}$$

Integrate

$$N_A \cdot dt = \frac{dz \cdot p_A}{M_A}$$

$$\frac{D_{AB}}{RT} \frac{dt}{z} \cdot \frac{P_T}{P_{Bm}} \cdot (P_{A1} - P_{A2}) = \frac{p_A}{M_A} dz$$

$$\int_{z_0}^{z_F} z dz = \int_0^{t_F} \frac{D_{AB} M_A}{RT p_A} \cdot \frac{P_T}{P_{Bm}} (P_{A1} - P_{A2}) dt$$

$$\Rightarrow \frac{1}{2}(z_F^2 - z_0^2) = \frac{D_{AB} M_A}{RT p_A} \cdot \frac{P_T}{P_{Bm}} (P_{A1} - P_{A2}) t_F$$

Rearrange

$$t_F = \frac{p_A (z_F^2 - z_0^2) \cdot RT}{2 D_{AB} M_A} \cdot \frac{P_{Bm}}{P_T} \cdot \frac{1}{(P_{A1} - P_{A2})}$$

Unit check

$$\frac{\frac{kg}{m^3} \cdot (m^2 - m^2) \cdot \frac{J}{kg \cdot mol \cdot K} \cdot k}{\frac{m^2}{s} \cdot \frac{kg}{kg \cdot mol}} \cdot \frac{1}{T} \cdot \frac{N}{m^2 - \frac{N}{m^2}}$$

$$\frac{1}{m} \cdot \frac{N \cdot m}{kg \cdot mol} \cdot \frac{s}{m^2} \cdot \frac{kg \cdot mol}{kg \cdot mol} \cdot \frac{m^2}{K}$$

Final unit S ✓

Example 4 Determine diffusivity w/ evaporation

(From Grisley 10-2)



tube $D = 0.01128 \text{ m}$

A CCl_3NO_2 (chloropicrin)
B air 1 atm

$t=0$ liquid from top = 0.0388 m

$t=1 \text{ day}$ $\dots = 0.0412 \text{ m}$

Vapor pressure ($P_{A1} = 3178.3 \text{ N/m}^2$)

$P_A = 1650 \text{ kg/m}^3$

$M_A = 164.39 \text{ kg/kg mol}$

Rearrange previous eq

$$\begin{cases} P_{A1} = 3178.3 \text{ N/m}^2 \\ P_{A2} = 0 \text{ N/m}^2 \\ P_{B1} = 101325 - 3178.3 \\ P_{B2} = 101325 \end{cases}$$

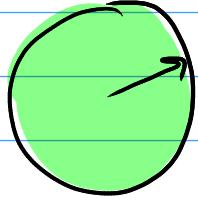
$$D_{AB} = \frac{P_A (z_F^2 - z_0^2) \cdot RT}{2t_f M_A} \cdot \frac{P_B m}{P_T} \cdot \frac{1}{(P_{A1} - P_{A2})} \quad P_B m = 99727.4$$

$$= \frac{1650 \cdot (0.0412^2 - 0.0388^2) \cdot 8314 \cdot 298}{2 \cdot 164.39 \cdot (3600 \cdot 24)} \cdot \frac{99727.4}{101325} \cdot \frac{1}{3178.3}$$

$$= 8.56 \times 10^{-6} \text{ m}^2/\text{s}$$

(assuming constant N_A then $D_{AB} = 8.75 \times 10^{-6} \text{ m}^2/\text{s}$)
+ 2.2% error

Example 6.2-4 Pseudo steady state through sphere

$r_i = 2.0 \text{ mm}$

 $T = 318 \text{ K}$
 $P_{A1} = 0.555 \text{ mm Hg}$
 $D_{AB} = 6.92 \times 10^{-6} \text{ m}^2/\text{s}$
 evaporation rate ?

Use stagnant B case eqn.

$$P_{A1} = 0.555 \text{ mm Hg} = 0.555 \times \frac{101325}{760} = 73.99 \text{ Pa}$$

$\therefore P_{B1}, P_{B2}$ very large

$$P_{Bm} \approx \frac{P_{B1} + P_{B2}}{2} = \frac{(101325 - 73.99) + 101325}{2} = 1.0129 \times 10^5 \text{ Pa}$$

$$\begin{aligned}
 N_A &= \frac{D_{AB}}{RT r_i} \cdot \frac{P_T}{P_{Bm}} (P_{A1} - P_{A2}) \\
 &= \frac{6.92 \times 10^{-6}}{8314 \cdot 318 \cdot 0.002} \cdot \frac{101325}{1.0129} \cdot (74 - 0) \\
 &= 9.68 \times 10^{-8} \text{ kg mol/m}^2/\text{s}
 \end{aligned}$$

Same setup of naphthalene sphere

generalize (r, radius, $P_A \ll P_T$)
density of solid ρ

- 1) Derive t_F for r decrease $r_i \rightarrow r_F$
- 2) Expression of t_F if $r_F = 0$ (fully evaporated)



Mass balance

$$\text{In} - \text{Out} + \text{Gen} = \text{Acc}$$

$$0 - \bar{N}_A + 0 = \frac{[4\pi \cdot r^2 \cdot \Delta r] \cdot \frac{\rho}{M_A}}{\Delta t}$$

$$\bar{N}_A = -4\pi r^2 \cdot \frac{\rho}{M_A} \cdot \frac{dr}{dt}$$

We have solution for \bar{N}_A ($P_{A1} \ll P_{Bm}$)

$$N_A = \frac{\bar{N}_A}{4\pi r^2} = \frac{D_{AB}}{RT} \frac{P_T}{P_{Bm}} (P_{A1} - P_{A2}) \cdot \frac{1}{r}$$

$$-\frac{4\pi r^2 \cdot \frac{\rho}{M_A}}{4\pi r^2} \cdot \frac{dr}{dt} = \frac{D_{AB} \cdot P_T}{RT \cdot P_{Bm}} (P_{A1} - P_{A2}) \frac{1}{r}$$

$$-r dr = \frac{D_{AB}}{RT} \cdot \frac{M_A}{\rho} \cdot \frac{P_T}{P_{Bm}} (P_{A1} - P_{A2}) dt$$

$$\int_{r_0}^{r_F} -r dr = \int_0 \frac{D_{AB}}{RT} \cdot \frac{M_A}{\rho} \cdot \frac{P_T}{P_{Bm}} (P_{A1} - P_{A2}) dt$$

$$\frac{(r_0^2 - r_F^2)}{2} = \frac{D_{AB}}{RT} \cdot \frac{M_A}{\rho} \cdot \frac{P_T}{P_{Bm}} (P_{A1} - P_{A2}) dt$$

$$\frac{(r_0^2 - r_F^2)}{2} = \frac{D_{AB}}{RT} \cdot \frac{M_A}{\rho} \cdot \frac{P_T}{P_{Bm}} (P_{A1} - P_{A2}) dt$$

$$t_F(r=r_F) = \frac{\rho RT P_{Bm}}{2 M_A D_{AB} P_T (P_{A1} - P_{A2})} \cdot \frac{1}{(r_0^2 - r_F^2)}$$

2) if $r_F = 0 \Rightarrow$

$$t_F(r=0) = \frac{\rho R T P_{Bm} r_0^2}{2 M_A D_{AB} P_T (P_{A1} - P_{A2})}$$

Complete evap

Compare with solution to example 3 in this note!

$$t_F = \frac{P_A (Z_F^2 - Z_0^2) \cdot RT}{2 D_{AB} M_A} \cdot \frac{P_{Bm}}{P_T} \cdot \frac{1}{(P_{A1} - P_{A2})}$$