

CHE 318 L06

Jan - 16 2026

Continue from L05 examples

### Example 6.3-2 (Geankoplis)

Diffusion of A  $\text{NH}_3$  in B water 278K 4.0mm thick  
at contact with organic liquid

Concentration of  $\text{NH}_3$  is constant equilibrium conc  
of  $\text{NH}_3$  at surface = 2.0 wt%  $\text{NH}_3$

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

$C_{\text{NH}_3}(\text{aq})$  the other end 1.0 wt%  $\rho = 961.7 \text{ kg/m}^3$

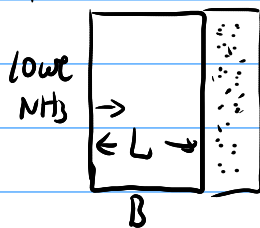
$$D_{AB} = 1.24 \times 10^{-9} \text{ m}^2/\text{s}$$

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

B)  $N_B$  ?

$\rho = 961.7$  2.0 wt%

We know from water-organic impermeability  
 $\Rightarrow N_B = 0$  Stagnant B



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

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

1. weight fraction  $\rightarrow$  molar fraction

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

$$x_B = 1 - x_A$$

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

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

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

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

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

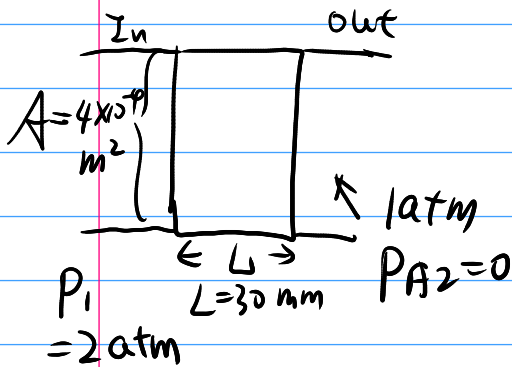
$$X_{A2} = \frac{\frac{0.02}{17.03}}{\frac{0.02}{17.03} + \frac{0.98}{18.02}} = 0.0211 \quad X_{B1} = 0.979$$

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

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

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

# Example 6.5.1 Diffusion through rubber (solubility)



total leakage of  $\text{CO}_2$  (amount / s)

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

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

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

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

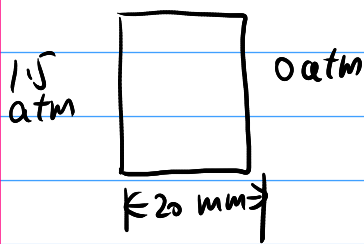
$$= \frac{0.11 \times 10^{-9} \times 0.90 \times (2 - 0)}{0.03 \times 22.414} \cdot 4.0 \times 10^{-4}$$

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

amount transferred / time

# Example 6.5-3

## Diffusivity vs permeability



Permeability

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

H<sub>2</sub>

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

$$S = 0.040$$

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

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

↳ same as  $D_{AB}$  table

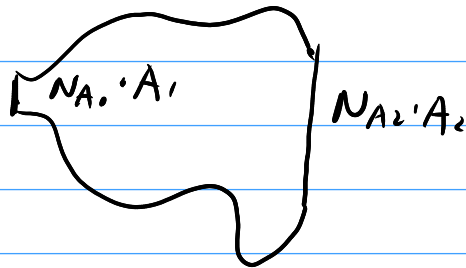
b) N<sub>2</sub> S.S.

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

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

# Diffusion through varying cross-section areas

Steady state :  $In \cdot Area_{in} - Out \cdot Area_{out} = 0$



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

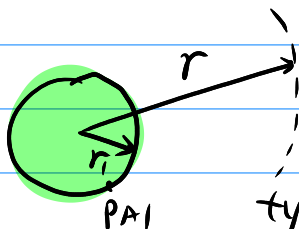
Can be used to solve diffusion through

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

Let  $\overline{N_A} = N_A \cdot A$

← mole/s      → 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)

Do not use the full solution for 1D! Use the ODE form

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

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

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

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

$\Downarrow$   
 Integrate

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

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

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

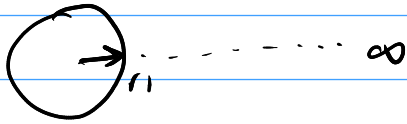
Conditions

- 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 equ. for some conditions

①  $r_2 \gg r_1$  ( $r_2 \rightarrow \infty$ )

example droplet evaporating / naphthalene sphere sublimation



Use the  $p_{Bm}$  term, we have

$$\frac{\overline{N_A}}{4\pi} \cdot \frac{1}{r_1} = \frac{D_{AB}}{RT} \frac{P_T}{p_{Bm}} (P_{A1} - P_{A2})$$

$$N_{A1} = \frac{\overline{N_A}}{4\pi r_1^2} = \frac{D_{AB}}{RT} \frac{P_T}{p_{Bm}} (P_{A1} - P_{A2}) \cdot \frac{1}{r_1}$$

(Do we have the correct unit?)

(looks like diffusion through sphere of radius  $r_1$   
has the same flux as through stagnant film with  
thickness =  $r_1$ )

If  $P_{A1} \ll P_T \Rightarrow p_{Bm} \approx P_T$

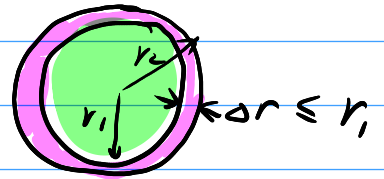
Use  $C_A$  form ( $P_A = C_A R T$ )

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

↪ more used in liquid

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

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



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

$\downarrow$   
 $\Delta r / r_1^2$

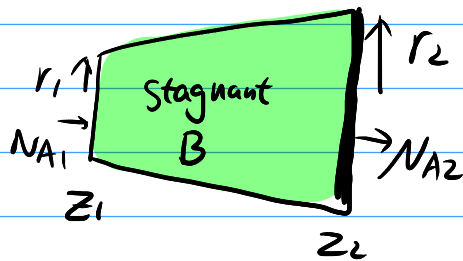
$$\frac{4\pi r_1^2 \cdot N_A}{4\pi} \cdot \frac{\Delta r}{r_1^2} = \frac{D_{AB} P_T}{RT P_{Bm}} (P_{A1} - P_{A2})$$

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

membrane thickness ! just like 1D  
stagnant B solution



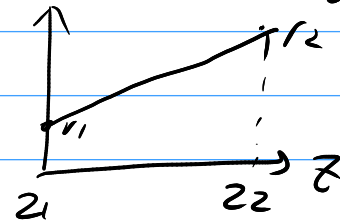
## Case 2 Diffusion through non-uniform area conduit



Again, use the ODE form of  $N_A$

$r(z)$  profile: linear

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



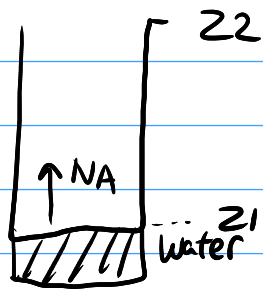
$$\frac{\overline{N_A}}{\pi r^2} = - \frac{D_{AB}}{RT} \frac{dp_A}{\left(1 - \frac{p_A}{p_T}\right)}$$

→ Solve

$$\frac{\overline{N_A}}{\pi} \int_{z_1}^{z_2} \frac{dz}{\left[ \left( \frac{r_2 - r_1}{z_2 - z_1} \right) z + r_1 \right]^2} = - \frac{D_{AB}}{RT} \int_{p_{A1}}^{p_{A2}} \frac{dp_A}{1 - \frac{p_A}{p_T}}$$

Can you solve this?

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



Water evaporates  $\rightarrow$  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)

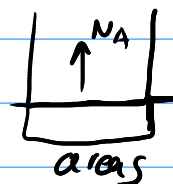
$$\text{at each } t \quad N_A = \frac{D_{AB}}{RT(z_2 - z_1)} \cdot \frac{P_T}{P_{Bm}} (P_{A1} - P_{A2})$$

$\downarrow$   $\downarrow$   $\swarrow$   
 $\frac{P_{B1} - P_{B2}}{\ln \frac{P_{B1}}{P_{B2}}}$  vapor pressure = 0 dry air

Mass balance

$$I_n - O_{ut} + Gen = Acc$$

$$0 - N_A + 0 = - \frac{(\text{mass loss})}{(\text{time})}$$



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

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

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

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

Final unit S ✓

# Example 4 Determine diffusivity w/ evaporation

(From Griskey 10-2)



tube  $D = 0.01128 \text{ m}$

A  $\text{CCl}_3\text{NO}_2$  (chloropicrin)

B air / atm

$t=0$  liquid from top =  $0.0388 \text{ m}$

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

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

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

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

Rearrange previous eq

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

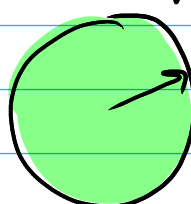
$$D_{AB} = \frac{\rho_A (z_F^2 - z_0^2) \cdot RT}{2z \cdot M_A} \cdot \frac{P_{Bm}}{P_T} \cdot \frac{1}{(P_{A1} - P_{A2})} \quad P_{Bm} = 99727.4$$

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

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

(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 equ.

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

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

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

$$N_A = \frac{D_{AB}}{RT r_i} \cdot \frac{P_T}{P_{Bm}} (P_{A1} - P_{A2}^{\infty}) \\ = \frac{6.92 \times 10^{-6}}{8314 \cdot 318 \cdot 0.002} \cdot \frac{101325}{101290} \cdot (74 - 0) \\ = 9.68 \times 10^{-8} \text{ kg mol/m}^2/\text{s}$$

Same setup of naphthalene sphere  
 generalize  $(r, \text{radius}, P_{A1} < P_T)$   
 density of solid  $\rho$

- 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

$$In - Out + Gen = Acc$$

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

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

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

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

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

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

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

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

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

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

2) if  $r_F = 0 \Rightarrow$

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

Complete evap

Compare with solution to example 3 in this note!

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