Mass Transfer-I

Molecular Diffusion in Fluids

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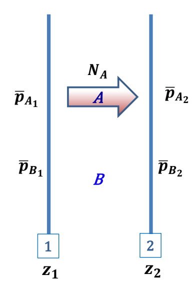
Molecular Diffusion in Gases

Steady state molecular diffusion of *A* through Non-Diffusing *B* (Binary gas mixture)

$$N_A = \frac{N_A}{N_A+N_B}\frac{D_{AB}}{z}\frac{p_t}{RT}\ln\frac{[N_A/(N_A+N_B)]p_t-\bar{p}_{A_2}}{[N_A/(N_A+N_B)]p_t-\bar{p}_{A_1}} \quad \text{.................(1)}$$



Diffusion of A through non-diffusing B

$$N_A = \text{Constant}, N_B = 0$$

$$\boxed{\frac{N_A}{N_A+N_B} = 1}$$

Equation (1) becomes

$$N_A = \frac{D_{AB}}{z}\frac{p_t}{RT}\ln\frac{p_t-\bar{p}_{A_2}}{p_t-\bar{p}_{A_1}} \quad \text{.................(2)}$$

Cont....

Since,

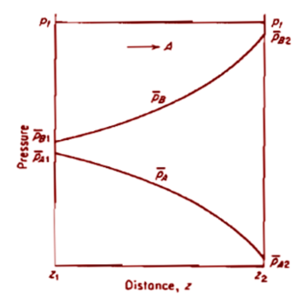
$$p_t-\bar{p}_{A_2} = \bar{p}_{B_2};\ p_t-\bar{p}_{A_1} = \bar{p}_{B_1};\ \bar{p}_{B_2}\text{-}\bar{p}_{B_1} = \bar{p}_{A_1}-\bar{p}_{A_2}$$

$$N_A = \frac{D_{AB}}{z}\frac{p_t}{RT}\frac{\bar{p}_{A_1}-\bar{p}_{A_2}}{\bar{p}_{B_2}-\bar{p}_{B_1}}\ln\frac{\bar{p}_{B_2}}{\bar{p}_{B_1}} \quad \text{.................(3)}$$

Considering the $\bar{p}_{B,M}$ as the log mean partial pressure difference of component B in between z_1 and z_2

$$\bar{p}_{B,M} = \frac{\bar{p}_{B_2}-\bar{p}_{B_1}}{\ln\ (\bar{p}_{B_2}/\bar{p}_{B_1})}$$

$$\boxed{N_A = \frac{D_{AB}}{RTz}\frac{p_t}{\bar{p}_{B,M}}(\bar{p}_{A_1}-\bar{p}_{A_2})} \quad \text{.................(4)}$$



Diffusion of A through Stagnant B

Steady state Equimolar Counter Diffusion (Binary gas mixture)

We know

$$N_A = (N_A + N_B)\frac{C_A}{C} - D_{AB}\frac{dC_A}{dz} \quad \text{.................(1)}$$

From ideal gas law,

$$\frac{C_A}{C} = \frac{\bar{p}_A}{P} = y_A \quad \text{and} \quad C_A = \frac{\bar{p}_A}{RT}$$

Putting in Eq. (1)

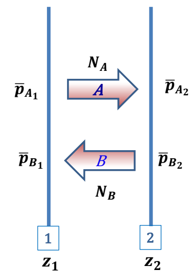
$$N_A = (N_A + N_B)\frac{\bar{p}_A}{P} - \frac{D_{AB}}{RT}\frac{d\bar{p}_A}{dz} \quad \text{.................(2)}$$

For Equimolar counter diffusion of A and B, *put* $N_A = -N_B$

$$\boxed{N_A + N_B = 0}$$

Then in Eq. (2)

$$N_A = -\frac{D_{AB}}{RT}\frac{d\bar{p}_A}{dz} \quad \text{.................(3)}$$



Cont….

$$N_A = -\frac{D_{AB}}{RT}\frac{d\bar{p}_A}{dz} \quad \text{.................(3)}$$

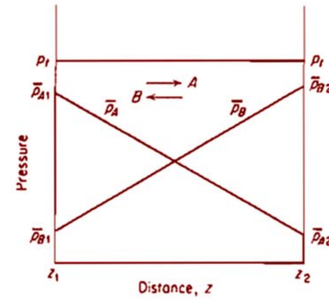
$$\int_{z_1}^{z_2} dz = -\frac{D_{AB}}{RT\,N_A}\int_{\bar{p}_{A_1}}^{\bar{p}_{A_2}} d\bar{p}_A \quad \text{.................(4)}$$

Integrating the Eq. (4)

$$z = -\frac{D_{AB}}{RT\,N_A}(\bar{p}_{A_1} - \bar{p}_{A_2}) \quad \text{.................(5)}$$

Rearranging the Eq. (5)

$$\boxed{N_A = -\frac{D_{AB}}{RTz}(\bar{p}_{A_1} - \bar{p}_{A_2})} \quad \text{.................(6)}$$



Equimolar Counter Diffusion

Example

Oxygen (A) is diffusing through carbon monoxide (B) under steady state conditions, with the carbon monoxide non-diffusing. The total pressure is $1x10^5\,\frac{N}{m^2}$ and the temperature is 0°C. The partial pressure of oxygen at two planes 2.0 mm apart is respectively, 13000 and 6500$\frac{N}{m^2}$. The diffusivity of the mixture is $1.87 \times 10^{-5}\frac{m^2}{s}$. Calculate the rate of diffusion of oxygen in $\frac{\text{kmol}}{s}$ through each square meter of the planes.

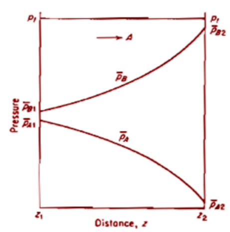
Solution:

Given:

$D_{AB} = 1.87 \times 10^{-5}\,\frac{m^2}{s}$
z = 0.002 m
R= 8314 $N.\,m/\,kmol.\,K$
T=273K;
$\bar{p}_{A1} = 13 \times 10^3$
$\bar{p}_{B1} = 10^5 - 13 \times 10^3 = 87 \times 10^3$
$\bar{p}_{A2}$=6500
$\bar{p}_{B2} = 10^5 - 6500 = 93.5 \times 10^3\,\frac{N}{m^2}$

For diffusion of ***A*** through non diffusing ***B***

$$N_A = \frac{D_{AB}}{RTz}\frac{p_t}{\bar{p}_{B,M}}(\bar{p}_{A_1} - \bar{p}_{A_2})$$



Cont….

$$N_A = \frac{D_{AB}}{RTz}\frac{p_t}{\bar{p}_{B,M}}(\bar{p}_{A_1} - \bar{p}_{A_2})$$

$$\bar{p}_{B,M} = \frac{\bar{p}_{B_2} - \bar{p}_{B_1}}{\ln(\bar{p}_{B_2}/\bar{p}_{B_1})} = \frac{(93.5-87)\times 10^3}{\ln(93.5/87)} = 90200\,\frac{N}{m^2}$$

$$N_A = \frac{(1.87 \times 10^{-5})(10^5)(13 - 6.5) \times 10^3}{8314(273)(0.002)(90.2 \times 10^3}$$

$$\boxed{N_A = 2.97 \times 10^{-5}\,\frac{kmol}{m^2.s}}$$

Molecular Diffusion in Liquids

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Molecular diffusion in Liquids

The general expression of molecular diffusion

$$N_A = \frac{N_A}{N_A + N_B}\frac{D_{AB}C}{z} ln\frac{N_A/(N_A+N_B) - C_{A_2}/C}{N_A/(N_A+N_B) - C_{A_1}/C}$$

Where:
ρ = Density
x_A = Mole fraction of A in liquid
M = Molecular weight

In case of liquid

$$C = \frac{n}{V} = \frac{weight/Molecular\ weight}{Volume} = \frac{weight/Volume}{Molecular\ weight} = \frac{Density}{Molecular\ weight} = \frac{\rho}{M}$$

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

The diffusion equation can be rewritten as

$$\boxed{N_A = \frac{N_A}{N_A + N_B}\frac{D_{AB}}{z}\left(\frac{\rho}{M}\right)_{av} ln\frac{N_A/(N_A+N_B) - x_{A_2}}{N_A/(N_A+N_B) - x_{A_1}}}$$

$$\left(\frac{\rho}{M}\right)_{av} = \frac{\left(\frac{\rho}{M}\right)_A + \left(\frac{\rho}{M}\right)_B}{2}$$

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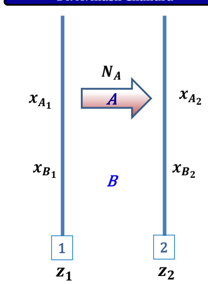
Steady state molecular diffusion in liquids

Diffusion of A through non-diffusing B $\quad N_A = \text{Constant}, N_B = 0$



$$\frac{N_A}{N_A + N_B} = 1$$

Then
$$N_A = \frac{D_{AB}}{z}\left(\frac{\rho}{M}\right)_{av} ln\frac{1 - x_{A_2}}{1 - x_{A_1}}$$

Since, $1 - x_{A_2} = x_{B_2}$; $1 - x_{A_1} = x_{B_1}$; $x_{B_2} - x_{B_1} = x_{A_1} - x_{A_2}$

Considering the $x_{B,M}$ as the log mean partial pressure difference of component B in between z_1 and z_2

$$x_{B,M} = \frac{x_{B_2} - x_{B_1}}{ln\ (x_{B_2}/x_{B_1})}$$

$$\boxed{N_A = \frac{D_{AB}}{z x_{B,M}}\left(\frac{\rho}{M}\right)_{av}(x_{A_1} - x_{A_2})}$$

$$\left(\frac{\rho}{M}\right)_{av} = \frac{1}{2}\left(\left(\frac{\rho}{M}\right)_1 + \left(\frac{\rho}{M}\right)_2\right)$$

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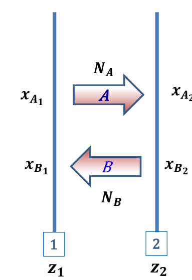
Cont.

For Equimolar counter diffusion of A and B

$$N_A = -N_B = Constant$$

$$\boxed{N_A + N_B = 0}$$



Similar to equimolar counter diffusion in gases

$$N_A = \frac{D_{AB}}{z}(C_{A_1} - C_{A_2})$$

$$\boxed{N_A = \frac{D_{AB}}{z}\left(\frac{\rho}{M}\right)_{av}(x_{A_1} - x_{A_2})}$$

Example

Calculate the rate of diffusion of Acetic acid (A) across a liquid film of non-diffusing water (B) solution 1 *mm* thick at 17 ^oC when the concentrations on opposite sides of the film are respectively 9 and 3 *wt.%* acid. The diffusivity of the acetic acid in the solution is $0.95 \times 10^{-9}\,\frac{m^2}{s}$. Density of 9% solution is 1012 *kg/m³* and 3% solution is 1003.2 *kg/m³.*

Solution:

Given:

$D_{AB} = 0.95.87 \times 10^{-9}\,\frac{m^2}{s}$

$z = 0.001\ m$

$M_A = 60.03$

$M_B = 18.02$

Density of 9% solution = 1012 kg/m^3

Density of 3% solution = 1003.2 kg/m^3

$$x_{A_1} = \frac{\frac{0.09}{60.03}}{\frac{0.09}{60.03} + \frac{0.91}{18.02}} = 0.0288 \qquad x_{B_1} = 1 - 0.0288 = 0.9712$$

Molecular weight of 9% solution

$$\frac{1}{M_1} = \frac{w_{A_1}}{M_A} + \frac{w_{B_1}}{M_B} = \frac{0.09}{60.03} + \frac{0.91}{18.02} = 0.0520$$

$$\boldsymbol{M_1 = 19.21\ kg/kmol}$$

Then

$$\left(\frac{\rho}{M}\right)_1 = \frac{1012}{19.21} = \mathbf{52.7}\ \boldsymbol{kg\ mol/m^3}$$

Cont….

Similarly for 3% solution $\quad x_{A_2} = 0.0092 \quad x_{B_2} = 0.9908$

$$M_2 = 18.40\ kg/kmol$$

$$\left(\frac{\rho}{M}\right)_2 = \mathbf{54.5}\ \boldsymbol{kg\ mol/m^3}$$

$$\left(\frac{\rho}{M}\right)_{av} = \frac{1}{2}(52.7 + 54.5) = 53.6\ \boldsymbol{kg\ mol/\ m^3}$$

Then

$$x_{B,M} = \frac{0.9908 - 0.9712}{ln\ (0.9908/0.9712)} = \mathbf{0.980}$$

$$\boldsymbol{N_A} = \frac{\boldsymbol{D_{AB}C}}{\boldsymbol{z x_{B,M}}}\left(\frac{\rho}{M}\right)_{av}(x_{A_1} - x_{A_2}) = \frac{0.95.87 \times 10^{-9}}{0.001 \times \mathbf{0.980}} \times \mathbf{53.6}\ (0.0288 - 0.0092) = \mathbf{1.018 \times 10^{-6}}\ \frac{\boldsymbol{kmol}}{\boldsymbol{m^2.s}}$$

$$\boxed{\boldsymbol{N_A = 1.018 \times 10^{-6}\ kmol/(m^2.s)}}$$

Unsteady state Diffusion

Unsteady State Diffusion

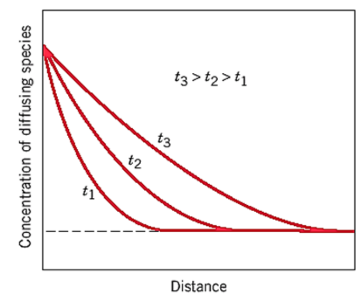
- The concentration of diffusing species is a function of both time and position $C = C(x, t)$
- In this case **Fick's Second Law** is used

Concentration changing with time : *Fick's second law*

$$\frac{\partial C_A}{\partial t} = -\frac{\partial J_A}{\partial x_A}$$

$$= D\frac{\partial^2 C_A}{\partial x_A^2}$$

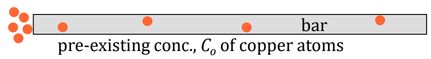
$$\boxed{\frac{\partial C_A}{\partial t} = D\frac{\partial^2 C_A}{\partial x_A^2}}$$



Example

Copper diffuses into a bar of aluminum.

Surface conc., C_S of Cu atoms

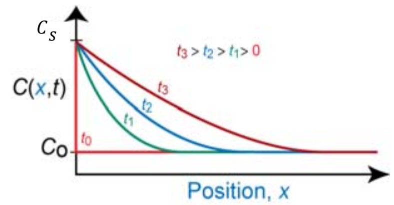


pre-existing conc., C_o of copper atoms

at $t = 0$, $C = C_o$ for $0 \le x \le \infty$

at $t > 0$, $C = C_S$ for $x = 0$ (constant surface conc.)

$C = C_o$ for $x = \infty$



Adapted from Fig. 5.5, *Callister & Rethwisch 8e*.

References

ETH

Mass Transfer

Theories for Mass Transfer Coefficients

Lecture 9, 15.11.2017, Dr. K. Wegner

- Lecture notes/ppt of Dr. Yahya Banat **(ybanat@qu.edu.qa)**