Mass Transfer

Fall 2024

Lecture #2

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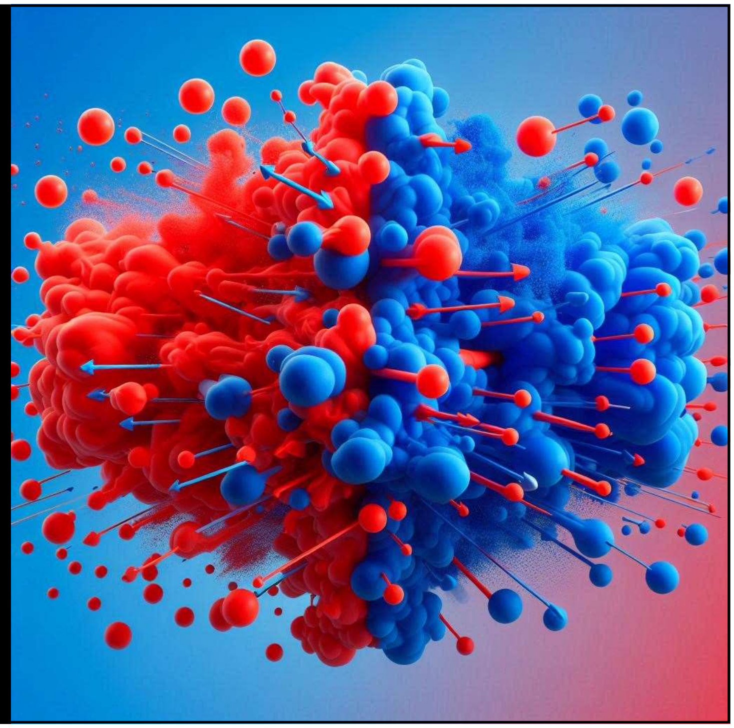
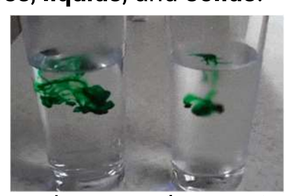


Diffusion

Diffusion is the process by which molecules move from an area of higher concentration to an area of lower concentration, driven by the concentration gradient. It occurs in **gases**, **liquids**, and **solids**.

Classification of Diffusion:



1. Molecular Diffusion (or Laminar Diffusion):

- Occurs due to random molecular motion in a medium.
- Directed by **Fick's Laws of Diffusion.**
- Happens naturally in gases, liquids, and solids where molecules spread out evenly over time.
  Example: The spreading of a perfume scent in a room, or a drop of ink in water.

2. Eddy Diffusion (or Turbulent Diffusion):

- This occurs in turbulent flows, where mixing happens due to eddies or swirls in the fluid.
- It is much faster than molecular diffusion because of the large-scale mixing.
  Example: The rapid mixing of dye in a turbulent river.

Molecular Diffusion is significant in stagnant or laminar flowing media, but not in turbulent media.

1.Molecular Diffusion (Laminar Diffusion)

Molecular Diffusion

Gas | **Liquid** | **Solid**

a) Equimolar ($N_A = -N_B$)

b) Diffusion of A in stagnant B ($N_B = 0$)

c) Diffusion through varying path

d) Diffusion through varying area

e) Diffusion of A and B plus Convection

f) Multicomponent diffusion

Molecular Diffusion

The basic Law of diffusion called "Fick's Law".

Molar Flux of A in B $\boxed{J_A \propto \frac{dC_A}{dZ}} \Rightarrow J_A = -D_{AB}\frac{dC_A}{dZ} = C_A \cdot u_A - C_A \cdot U$ --------------- (1)

where D_{AB} = diffusion coefficient or diffusivity of A in B, it is a physical property $(\frac{m^2}{sec})$

C_A = molar concentration of A in $(\frac{Kmol}{m^3})$

Z = Distance in the direction of diffusion (m)

U = Molar average velocity $= \left(\frac{1}{C_t}\right) \cdot \sum C_i \cdot u_i$

For the case of A diffusing in B

$U = \frac{1}{C_t}(C_A \cdot u_A + C_B \cdot u_B)$ sub in (1)

$$-D_{AB}\frac{dC_A}{dZ} = C_A \cdot u_A - C_A \cdot \frac{1}{C_t}(C_A \cdot u_A + C_B \cdot u_B)$$

$$-D_{AB}\frac{dC_A}{dZ} = N_A - \frac{C_A}{C_t}(N_A + N_B) \Rightarrow \boxed{N_A = \frac{C_A}{C_t}(N_A + N_B) - D_{AB}\frac{dC_A}{dZ}} \text{ --- (2)}$$

Bulk Flow | Molecular Diffusion

Molecular Diffusion

For gases

$P = C.R.T \Rightarrow C_t = \frac{P_t}{R.T}$; $C_A = \frac{P_A}{R.T}$ Sub in (2)

$$N_A = \frac{\frac{P_A}{R.T}}{\frac{P_t}{R.T}} (N_A + N_B) - D_{AB} \frac{d\frac{P_A}{R.T}}{dZ}$$

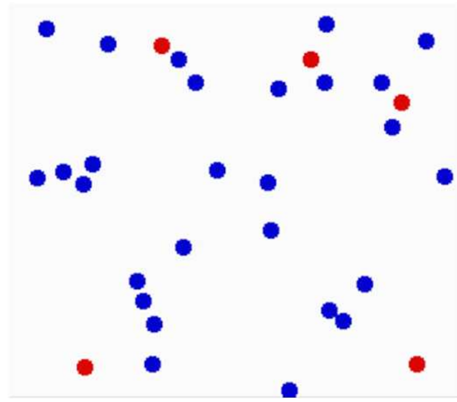
$$N_A = \frac{P_A}{P_t} (N_A + N_B) - \frac{D_{AB}}{R.T} . \frac{dP_A}{dZ} \text{------------ (3)}$$

$P_A = P_t . y_A \Rightarrow y_A = \frac{P_A}{P_t}$ sub in (3)

$$N_A = y_A (N_A + N_B) - \frac{D_{AB} . P_t}{R.T} . \frac{dy_A}{dZ}$$

$$\boxed{N_A = y_A (N_A + N_B) - D_{AB} . C_t . \frac{dy_A}{dZ}} \text{-------- (4)}$$

Bulk Flow Molecular Diffusion



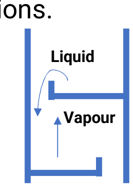
Molecular Diffusion

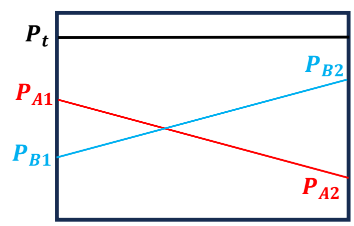
a) Counter diffusion (*i*- equimolar & *ii*- non-equimolar)

Species A and B diffuse in each other but in opposite directions.

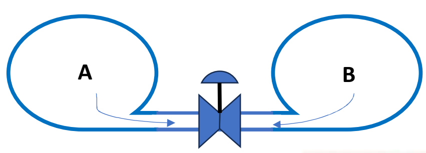
Examples of Counter Diffusion:

- Vapor and liquid in a distillation column.

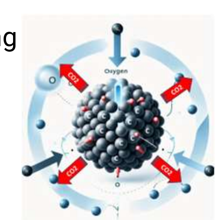




- Two tanks connected.



- Oxygen diffuses into carbon particles producing carbon dioxide which diffuses back.



حالات

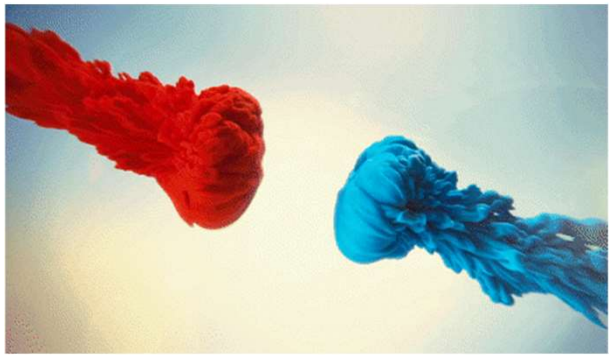
لمادتين ينتشران بعكس الاتجاه

- برج تقطير
- كرة كاربونية
- خزانين مربوطة
- تُذكر في السؤال

Molecular Diffusion

a) *i*- Equimolar ($N_A = -N_B$)

A and B diffuse at equal rates in opposite directions.



$$N_A = \frac{P_A}{P_t}(N_A + N_B) - \frac{D_{AB}}{R.T} \cdot \frac{dP_A}{dZ} \text{------------ (3)}$$

$N_A = -N_B$ sub in (3)

$$N_A = \frac{P_A}{P_t}((-N_B) + N_B) - \frac{D_{AB}}{R.T} \cdot \frac{dP_A}{dZ}$$

$$N_A = -\frac{D_{AB}}{R.T} \cdot \frac{dP_A}{dZ}$$

By integration

$$\boxed{N_A = -\frac{D_{AB}}{R.T} \cdot \frac{P_{A2} - P_{A1}}{Z_2 - Z_1}}$$ (Laminar Flow – Gas – Equimolar)

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Molecular Diffusion

a) *i*- Equimolar ($N_A = -N_B$)

Example 2 : Prove that for equimolar diffusion D_{AB} = D_{BA}

Solution

for equimolar $N_A = -N_B$ -----(*)

$$N_A = \frac{P_A}{P_t}((-N_B) + N_B) - \frac{D_{AB}}{R.T} \cdot \frac{dP_A}{dZ} \Rightarrow N_A = -\frac{D_{AB}}{R.T} \cdot \frac{dP_A}{dZ} \text{-----(**)}$$

$$N_B = \frac{P_B}{P_t}((-N_B) + N_B) - \frac{D_{BA}}{R.T} \cdot \frac{dP_B}{dZ} \Rightarrow N_B = -\frac{D_{BA}}{R.T} \cdot \frac{dP_B}{dZ} \text{-------(***)}$$

Sub (**) & (***) in (*)

$$-\frac{D_{AB}}{R.T} \cdot \frac{dP_A}{dZ} = +\frac{D_{BA}}{R.T} \cdot \frac{dP_B}{dZ} \text{-----(****)} \; ; P_t = P_A + P_B \Rightarrow dP_t = dP_A + dP_B = 0 \Rightarrow dP_A = -dP_B$$

sub ($dP_A = -dP_B$) in (****)

$$+\frac{D_{AB}}{R.T} \cdot \frac{dP_B}{dZ} = +\frac{D_{BA}}{R.T} \cdot \frac{dP_B}{dZ} \Rightarrow \boxed{D_{AB} = D_{BA}}$$

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Example 3 : A uniform tube (0.1) m long and (0.01) m inside diameter containing Nitrogen gas. Ammonia gas is diffusing through the pipe. At point (1), $\boldsymbol{P_{A1} = 1.013 * 10^4\ Pa}$, and at point (2) $\boldsymbol{P_{A2} = 0.507 * 10^4\ Pa}$. The total pressure is $\boldsymbol{P_t = 1.013 * 10^5\ Pa}$, and the diffusivity $\boldsymbol{D_{AB} = 0.2 * 10^{-4} \frac{cm^2}{sec}}$.

Calculate: 1) Fluxes of (A) and (B) at temperature = 298K. 2) The rate of molar transfer for (A) & (B).

Solution

$\boldsymbol{P_{A1} = 1.013 * 10^4\ Pa}$
$\boldsymbol{P_{B1} = 1.013 * 10^5 - P_{A1}}$
$\boldsymbol{Z_1 = 0\ m}$

$\boldsymbol{P_{A2} = 0.507 * 10^4\ Pa}$
$\boldsymbol{P_{B2} = 1.013 * 10^5 - P_{A2}}$
$\boldsymbol{Z_2 = 0.1\ m}$

1) The system is closed at constant Temperature and pressure, So the diffusion follow equimolar ($\boldsymbol{N_A = -N_B}$)

$$N_A = -\frac{D_{AB}}{R.T} \cdot \frac{P_{A2} - P_{A1}}{Z_2 - Z_1} \quad \Rightarrow \quad N_A = -\frac{0.23*10^{-4}}{8.314*298} \cdot \frac{0.507*10^4 - 1.013*10^4}{0.1 - 0.0} = 4.7 * 10^{-7} \frac{Kmol}{m^2.Sec}$$

For (B) $\boldsymbol{P_{B1} = P_t - P_{A1}}$; $\boldsymbol{P_{B2} = P_t - P_{A2}}$; $\boldsymbol{D_{AB} = D_{BA}}$

$$N_B = -\frac{D_{BA}}{R.T} \cdot \frac{P_{B2} - P_{B1}}{Z_2 - Z_1} = -4.7 * 10^{-7} \frac{Kmol}{m^2.Sec}$$

Example 3 :

Solution

2) The rate of molar transfer for (A) & (B).

The rate of molar transfer of (A) = $\boldsymbol{r_A}$

$$\boldsymbol{N_A = \frac{r_A}{area} \quad \Rightarrow r_A = N_A \cdot Area}$$

$$= 4.7 * 10^{-7} \cdot \frac{\pi}{4} \cdot (0.01)^2 = 36.66 * 10^{-12} \frac{Kmol}{Sec}$$

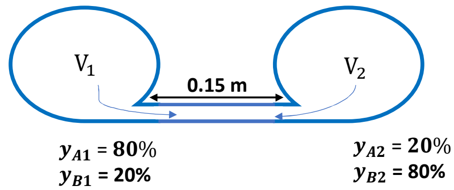
$$\boldsymbol{r_B = N_B \cdot Area} = -36.66 * 10^{-12} \frac{Kmol}{Sec}$$

What if the question asked about Mass Transfer rate for A and B ?

Example 4 : Two large vessels are connected as shown below. Vessel (1) contains 80% N_2 (A) and 20% O_2 (B). Vessel (2) contains 20% N_2 (A) and 80% O_2 (B). The temperature and the total pressure are (20 ℃) and (2 atm). Calculate:

- The flux and rate of transport of N_2 and O_2 from vessel 1 to vessel 2.
- The partial pressure of N_2 in the tube (0.05 m) from vessel (1) .
- Th net molar flux (N_{net}).

Given that diffusivity of $N_2 - O_2$ is 1.01*10^{-5} $\frac{m^2}{sec}$.



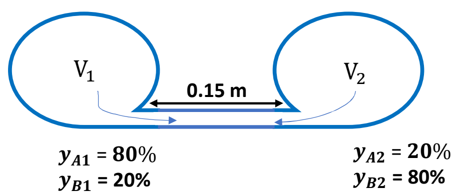
Solution

1) Closed System, So the diffusion follow equimolar ($\boldsymbol{N_A = -N_B}$)

$$N_A = -\frac{D_{AB}}{R.T} \cdot \frac{P_{A2} - P_{A1}}{Z_2 - Z_1}$$

Example 4 :

Solution



1) $P_{A1} = P_t * y_{A1} \Rightarrow P_{A1} = 2 \text{ atm} * 0.8 = 1.6 \text{ atm}$

$P_{A2} = P_t * y_{A2} \Rightarrow P_{A2} = 2 \text{ atm} * 0.2 = 0.4 \text{ atm}$

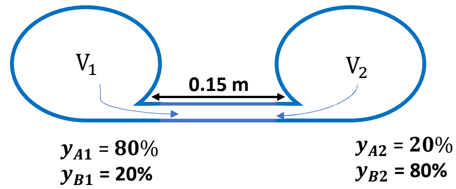
$P_{B1} = P_t - P_{A1}$; $P_{B2} = P_t - P_{A2}$

$P_{B1} = 2 - 1.6 = 0.4 \, atm$; $P_{B2} = 2 - 0.4 = 1.6 \, atm$

$$N_A = -\frac{1.01*10^{-5}}{0.082*293} \cdot \frac{0.4-1.6}{0.15-0} = 3.3*10^{-6} \frac{kmol}{m^2.sec} \; ; \; N_B = -N_A = -3.3*10^{-6} \frac{kmol}{m^2.sec}$$

Example 4 :

Solution



2) Partial pressure of N_2 *(P_A)*

The pressure change is linear between 1 and 2

$$dP_A /dZ = \frac{P_{A2} - P_{A1}}{Z_2 - Z_1} = \frac{0.4-1.6}{0.15-0} = -8 \text{ atm/m}$$

At $Z = 0.05\ m$

$$dP/dZ = \frac{P_A - P_{A1}}{Z - Z_1} = \frac{P_A - 1.6}{0.05 - 0} = -8 \text{ atm/m} \Rightarrow P_A = 1.2 \text{ atm}$$

3) Th net mass flux

$$N_{net} = N_A . Mwt_A + N_B . Mwt_B$$

$$= 3.3 * 10^{-6} * 28 + (-3.3 * 10^{-6}) * 32 \Rightarrow N_{net} = -1.344 * 10^{-5} \frac{kg}{m^2 .sec}$$

HW 2: Due Date Saturday, October 19th

Q1

A tube of length 1 m separates two chambers. One chamber contains pure oxygen (O_2) at a pressure of 1 atm, and the other contains pure nitrogen (N_2) at a pressure of 1 atm. The gases diffuse through the tube, and the system operates under steady-state conditions with equimolar counter-diffusion.
The diffusion coefficient for O_2 in N_2 is D_{AB}=2.0 $* 10^{-5}$ m^2/sec at 298 K.
Calculate the molar flux of oxygen, using the linear form of Fick's first law.

Solution

=8.18 $* 10^{-5}$ mol/ m^2.sec

Q2

Consider a binary gas mixture of species A and B undergoing non-equimolar counter-diffusion in a long tube. Species A is diffusing to the right at a rate **three times** faster than species B which is diffusing to the left. The total pressure is constant, and the system is isothermal at temperature T. **Derive** the equation for the molar flux of species A.

Solution

$$N_A = -\frac{3D_{AB}}{2RT}\frac{P}{z_2 - z_1}\ln\left(\frac{1-\frac{2}{3}\frac{P_{A2}}{P}}{1-\frac{2}{3}\frac{P_{A1}}{P}}\right)$$