THAPAR INSTITUTE
OF ENGINEERING & TECHNOLOGY
(Deemed to be University)

# Mass Transfer-I

## Diffusion

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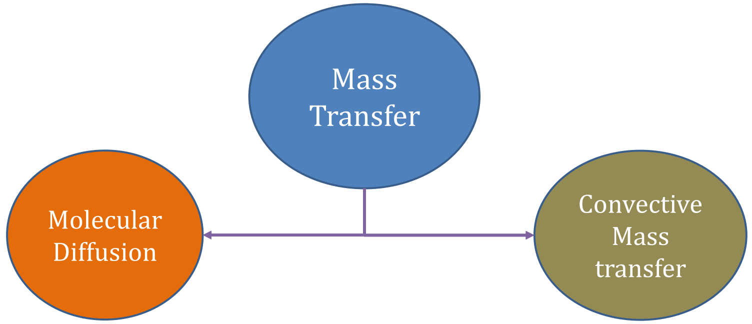
## Modes of mass transfer



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# Molecular Diffusion

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**Molecular Diffusion - Mass transport by atomic motion**

**Mechanisms**

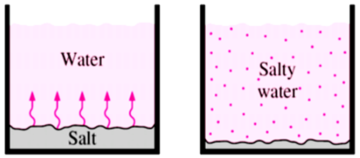
- Gases & Liquids – random (Brownian) motion
- Solids – vacancy diffusion or interstitial diffusion

**Diffusion of molecules happens due to a concentration gradient.**

**Diffusion is a passive process which means that no energy is needed.**

## Cont…

- Whenever there is concentration difference in a medium, nature tends to equalize things by forcing a flow from the high to the low concentration region.




Before After

- The molecular transport process of mass is characterized by the general equation:

***Rate of transfer process = driving force / resistance***





## Concentration, Velocity and Flux

The Concentration of a species in a solution is expressed in terms of one of the following

$$\sum_{i=1}^{n} \rho_i = \rho; \quad \sum_{i=1}^{n} C_i = C; \quad \sum_{i=1}^{n} w_i = 1; \quad \sum_{i=1}^{n} x_i = 1$$

$\rho_i =$ mass concentration of the species $i$ in kg/$m^3$
$\rho =$ total mass concentration of all the species in a solution in kg/$m^3$
$w_i = \frac{\rho_i}{\rho} =$ mass concentration of the species $i$ in a solution
$C_i =$ molar concentration of the species $i$ in a solution in kmol/ $m^3$
$x_i = \frac{C_i}{C} =$ mole fraction of the species $i$ in a solution
$n$ is the number of species in a solution

In gas mixture the concentration of species in gas is expressed in terms of partial pressure p, or mole fraction $y_i = \frac{p_i}{P}$, mole fraction of species 1 in a solution is $x_i$





## Diffusion velocities

### Mass Average velocities

In n component mixture mass average velocity

$$u = \frac{\sum_{i=1}^{n} \rho_i u_i}{\sum_{i=1}^{n} \rho_i} = \frac{1}{\rho} \sum_{i=1}^{n} \rho_i u_i$$

$u_i$ is the linear velocity of the $i^{th}$ species in the concerned direction. $u_i$ does not mean the instantaneous velocity of a molecule of the component.

### Molar Average Velocity

The molar average velocity of a mixture

$$U = \frac{\sum_{i=1}^{n} C_i u_i}{\sum_{i=1}^{n} C_i} = \frac{1}{C} \sum_{i=1}^{n} C_i u_i$$





## Mass flux

Relative to a stationary observer: $\boldsymbol{n_i}$ $\boxed{\boldsymbol{n_i = \rho_i v_i}}$

Relative to an observation moving with the mass average velocity: $\boldsymbol{i_i}$ $\boxed{\boldsymbol{i_i = \rho_i (u_i - u)}}$

Relative to an observer moving with the molar average velocity: $\boldsymbol{j_i}$ $\boxed{\boldsymbol{j_i = \rho_i (u_i - U)}}$

## Molar flux

Relative to a stationary observer: $\boldsymbol{N_i}$ $\boxed{\boldsymbol{N_i = C_i v_i}}$

Relative to an observation moving with the mass average velocity: $\boldsymbol{I_i}$ $\boxed{\boldsymbol{I_i = C_i (u_i - u)}}$

Relative to an observer moving with the molar average velocity: $\boldsymbol{J_i}$ $\boxed{\boldsymbol{J_i = C_i (u_i - U)}}$

## Example ( Calculation of average velocities)

**A gas mixture ($N_2 = 5\%, H_2 = 15\%, NH_3 = 76\%$ and $Ar$ =4%) flows through a pipe, 25.4 mm in diameter, at 4.05 bar total pressure. If the velocities of the respective components are 0.03m/s, 0.065 m/s, 0.03 m/s and 0.02 m/s, Calculate the mass average and volume average velocities of the mixture.**

### Solution

Let us consider $\boldsymbol{N_2}$ as the **1st** component, $\boldsymbol{H_2}$ as the **2nd** component, $\boldsymbol{NH_3}$ is the **3rd** component, $\boldsymbol{Ar}$ is the **4th** component.

The volume average velocity (molar average velocity) $U = \frac{1}{C}(C_1u_1 + C_2u_2 + C_3u_3 + C_4u_4)$

$y_i$ is the mole fraction of component $i$ in the gas mixture. Putting the values we get,

$$U = (0.05)(0.03) + (0.15)(0.035) + (0.76)(0.03) + (0.04)(0.02)$$
$$=0.0303 \text{ m/s}$$





## cont...

The mass average velocity is

$$U = \frac{1}{\rho}(\rho_1u_1 + \rho_2u_2 + \rho_3u_3 + \rho_4u_4)$$

$\rho_i$= mass concentration of the species I in kg/$m^3$
$\rho$= total mass concentration of all the species in a solution in kg/$m^3$
$M_i$ = molecular weight of the $i^{th}$ component
$M$= Average molecular weight of the mixture

$$\rho_i = \frac{p_i}{RT}M_i$$

$$\rho = \frac{P}{RT}M$$

$$\frac{\rho_i}{\rho} = \frac{p_i}{p}\frac{M_i}{M} = y_i\frac{M_i}{M}$$

$$M = y_1M_1 + y_2M_2 + y_3M_3 + y_4M_4 = (0.05)(28) + (0.15)(2) + (0.76)(17) + (0.04)(40)$$
$$= 16.22$$

$$U = \frac{1}{M}\sum_{i=1}^{4} y_i\frac{M_i}{M} = (0.05)(28)(0.03) + (0.15)(2)(0.035) + (0.76)(17)(0.03) + (0.04)(40)(0.02)$$
$$= 0.029\ m/s$$



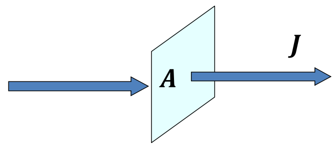


## The rate of diffusion

**The rate of diffusion** at which a solute moves at any point in any direction depend on concentration gradient. The rate of diffusion is conveniently described in terms of molar flux, mole/ (area) (time). The area being measured in a direction normal to the diffusion.

- Rate of diffusion increases with decreasing pressure
- Rate of diffusion increases with increasing temperature(increasing temperature increases the molecular velocity)

$$\boldsymbol{J = \frac{M}{At}}$$








## Diffusion Flux

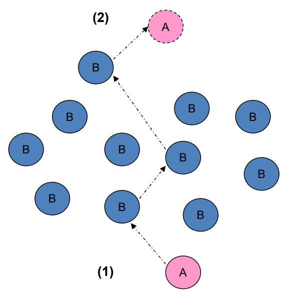
**Flux of diffusing atoms, $J$**

$$J \equiv \text{Flux} \equiv \frac{\text{moles (or mass) diffusing}}{\text{(surface area)(time)}} = \frac{mol}{cm^2 s} \text{ or } \frac{kg}{m^2 s}$$

**Number of atoms diffusing through unit area per unit time [atoms/($m^2$s)]**
**or**
**Mass of atoms diffusing through unit area per unit time [kg/($m^2$ s)]**

## Fick's Law of Diffusion (Steady-state Diffusion)

- Molecular diffusion or molecular transport can be defined as the transfer or movement of individual molecules through a fluid by mean of the random, individual movements of the molecules.
- If there are greater number of A molecules near point (1) than at (2), then since molecules diffuse randomly in both direction, more A molecules will diffuse from (1) to (2) than from (2) to (1).
- The net diffusion of A is from high to low concentration regions.
- Diffusion raises due to Brownian motion in molecules
- Molecules move from higher concentration zone to lower concentration zone until equilibrium is established.
- Rate of diffusion is independent of time but dependent on concentration gradient.




**Steady State Diffusion flux does not change with time**

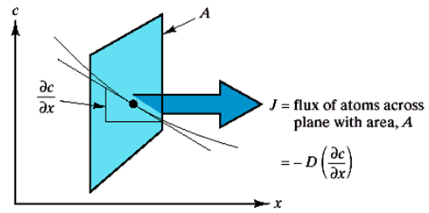




## Fick's first law:

$$J \propto \frac{dC}{dx}$$

$$J = -D\frac{dC}{dx}$$




**D = diffusion coefficient**

**Concentration gradient is *'driving force'***

**Minus sign means diffusion is 'downhill': toward lower concentrations**

- **Diffusion flux does not change with time**
- **Concentration profile: Concentration *(kg/m³)* vs. position**
- **Concentration gradient*:* *dC/dx (kg / m⁴)***





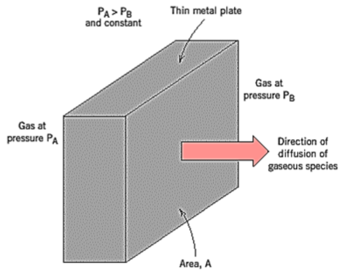
## Fick's 1st Law of Diffusion

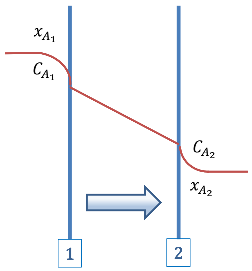
Mass transfer flux is proportional to concentration gradient $\frac{dC_A}{dz}$

$$J^*_{AZ} \propto -\frac{dc_A}{dz}$$

$$J^*_{AZ} = -D_{AB}\frac{dc_A}{dz}$$

$$\boxed{J^*_{AZ} = -cD_{AB}\frac{dx_A}{dz}}$$




$J^*_{AZ}$ is the molar flux of component A in the z-direction in *kg mol A/s.m²*
$D_{AB}$ is the molecular diffusivity of the molecule A in B in *m²/s*
$c_A$ is the concentration of A in *kg mol/m³*
$z$ is the distance of diffusion in *m*
$c$ total concentration of A and B *[kgmol (A + B)/m³]*
$x_A$ mole fraction of A in the mixture of A and B

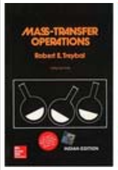


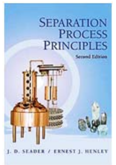


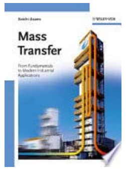
## Other Diffusion phenomena

- **Thermal diffusion:** Diffusion due to a temperature gradient. Usually negligible unless the temperature gradient is very large.
- **Pressure diffusion:** Diffusion due to a pressure gradient. Usually negligible unless the pressure gradient is very large.
- **Forced diffusion:** Diffusion due to external force field acting on a molecule. Forced diffusion occurs when an electrical field is imposed on an electrolyte ( for example, in charging an automobile battery)
- **Knudsen diffusion:** Diffusion phenomena occur in porous solids.

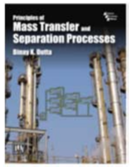
## References

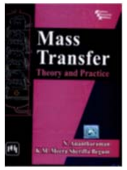


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Mass Transfer

Theories for Mass Transfer Coefficients

Lecture 9, 15.11.2017, Dr. K. Wegner

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