Introduction
Diffusion concepts

Examples, definitions and diffusion
Laws

Objectives

- Define mass transfer and its relation to transport phenomena.
- Diffusion of molecules.
- Types of diffusion.
- Examples and applications of mass transfer.
- Fick's law in mass transfer.
- Diffusion coefficient.

Transport Phenomena
Definition

Transport phenomena include three types of transfer:

(1) Momentum transfer

Fluid mechanics like fluid flow, mixing, sedimentation.

The interest is in the transfer of momentum.

(2) Heat Transfer

Conduction of heat, convection, evaporation, distillation, drying.

The interest is in the transfer of energy.

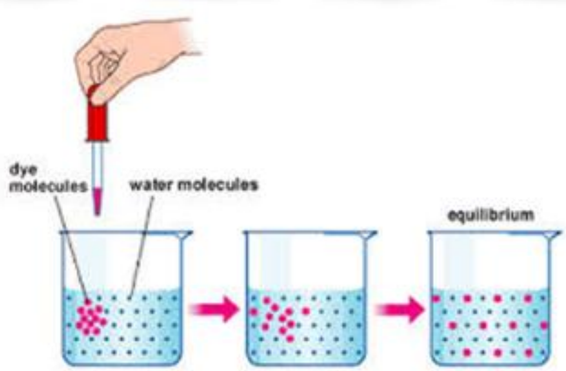
(3) Mass Transfer

Membrane processes, crystallization, evaporation, distillation, drying.

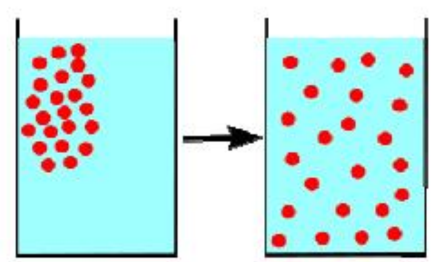
The interest is in the transfer of molecules or material.

Examples of Mass Transfer

Dye distribution in a liquid:

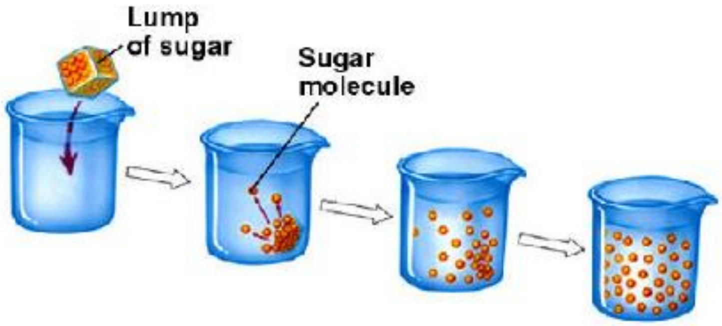


This process is called **Diffusion** of the dye in the water.



Examples of Mass Transfer

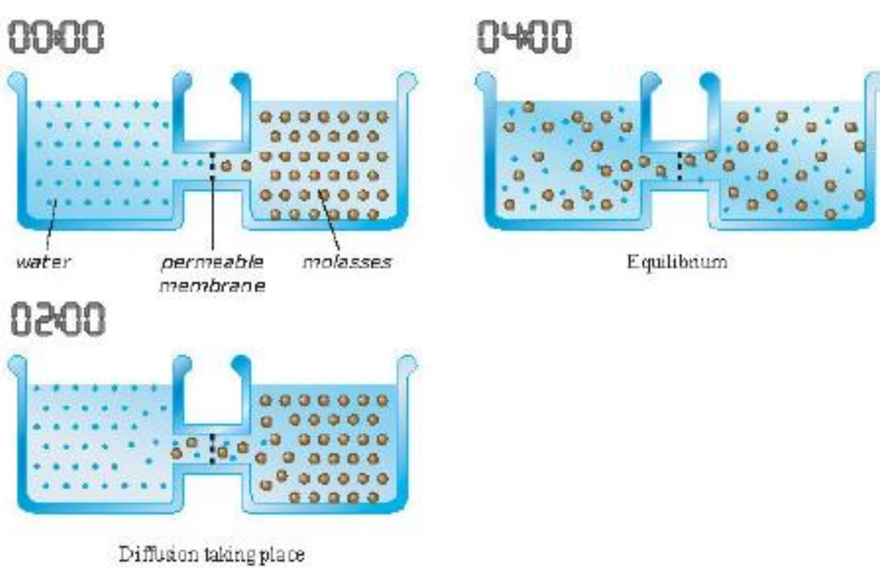
Dissolution of sugar or salt in water:



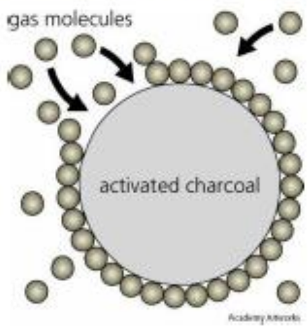
This process is again called **Diffusion**.

Examples of Mass Transfer

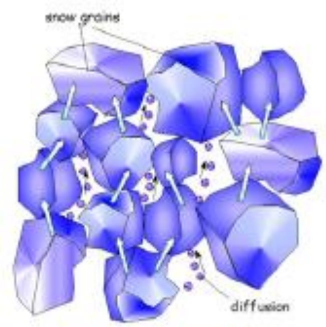
Diffusion of gas, liquid or solid through a membrane:



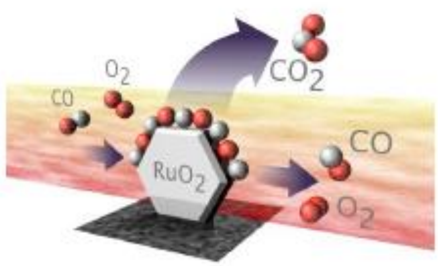
Application of Mass Transfer



adsorption

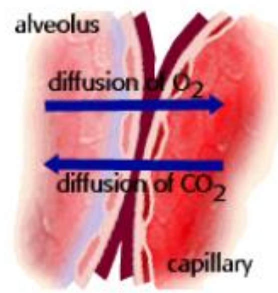


crystallization



catalysis

Breathing

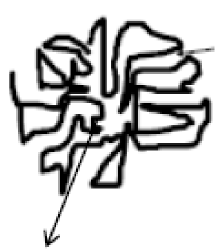


Inhaling of O2 and exhale of CO2 as gas exchange between lungs and blood capillaries

Application of Mass transfer

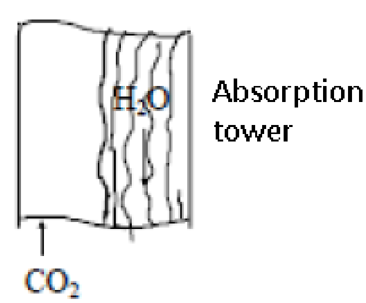
Reaction in porous catalyst

C2H6 → C2H4 + H2



Reactants or products diffuse in or out of porous catalysts pellet

Absorption of CO2 by Water

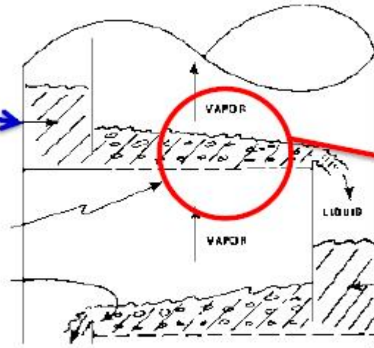


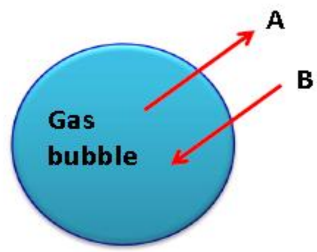
What is the flux of CO_2 on the water surface?

Application of Mass transfer

Distillation columns
e.g., in petroleum refinery

Species exchange between
gas-liquid around the trays





This mass transfer enriches
species (A) in the liquid, and
species (B) in the gas

All transport processes are characterized by the same general type of equation:

$$\text{rate of transfer} = \frac{\text{driving force}}{\text{resistance}}$$

$$\text{rate of transfer} = -\delta A \frac{\Delta \Gamma}{\Delta z}$$

Momentum Transfer	Heat Transfer	Mass Transfer
$\tau = -\mu A \frac{\Delta u}{\Delta z}$	$Q = -k A \frac{\Delta T}{\Delta z}$	$J = -D A \frac{\Delta ?}{\Delta z}$

Mass Transfer

Mass transfer occurs whenever there is a **gradient in the concentration** of a species.

$$J = -DA\frac{\Delta C}{\Delta z}$$

Mass transfer may occur in a gas mixture, a liquid solution or solid.

The basic mechanisms are the same whether the phase is a gas, liquid, or solid.

Fick's law:

Mass diffusion: Linear relation between the rate of diffusion of chemical species and the concentration gradient of that species.

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

Thermal diffusion: Diffusion due to a temperature gradient.

Pressure diffusion: Diffusion due to a pressure gradient.

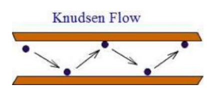
Types of diffusion:

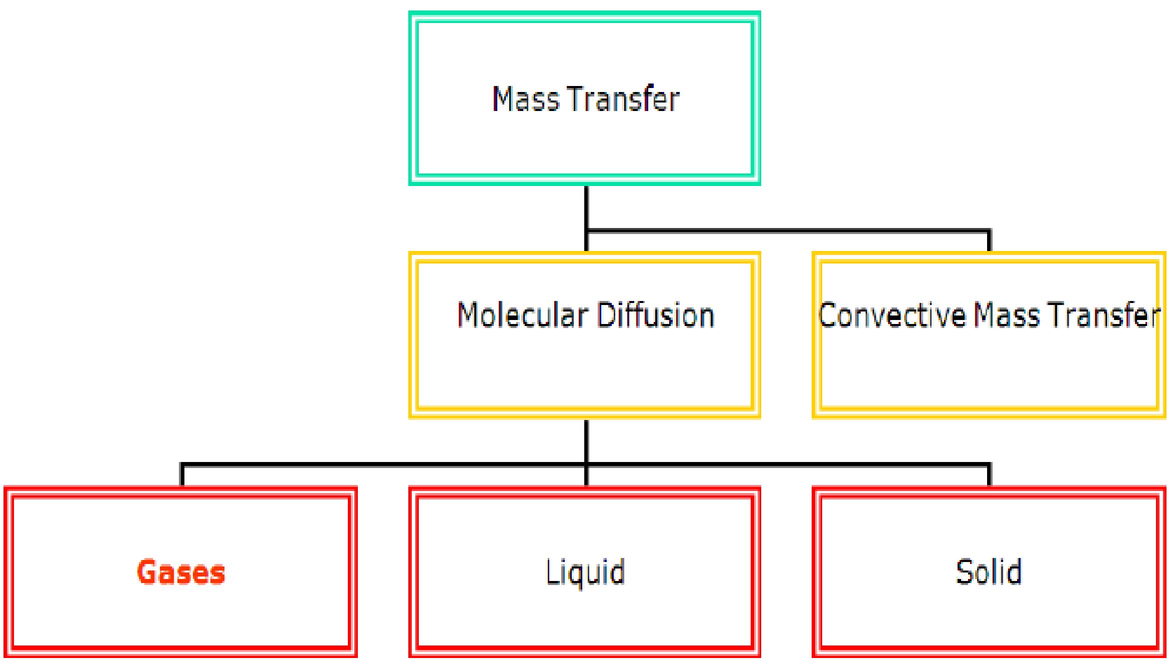
(1) **Free diffusion**: when species move freely.

(2) **Forced diffusion**: Diffusion due to external force acting on a molecule.

Forced diffusion occurs when an electrical field is imposed on an electrolyte (for example, in charging an automobile battery)

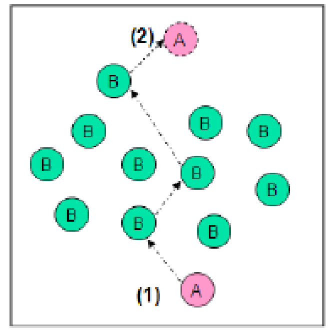
(3) **Knudsen diffusion**: Diffusion through a porous solid.





Diffusion

$$J^*_{A_Z} = -D_{AB}A\frac{dC_A}{dz}$$



J^*_A is the molar flux of component A in the z direction in kg mol A/s.

D_{AB} is the molecular diffusivity of the molecule A in B in m^2/s.

C_A is the concentration of A in kg mol/m^3.

z is the distance of diffusion in m

Definition of concentration

- **Number of molecules** of a species present per unit volume (molecules/m^3)

- **Molar concentration** of species *i* = Number of moles of *i* per unit volume (kmol/m^3)

- **Mass concentration =** Mass of *i* per unit volume (kg/m^3)

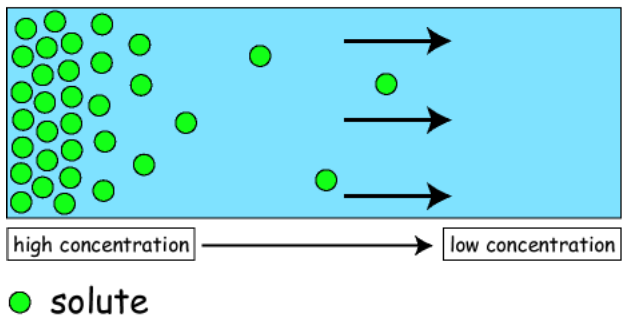
SUMMARY

Based on Observations

- Mass transfer by ordinary molecular diffusion occurs because of a difference in concentration or gradient; that is, a species diffuses in the direction of decreasing concentration.
- The mass-transfer rate is proportional to the area normal to the direction of mass transfer and not to the volume of the mixture. Thus, the rate can be expressed as a flux.
- Net mass transfer stops when concentrations are uniform.

Driving forces for Diffusion

- **Possible driving forces (gradients) for Diffusion**
  1. Ordinary diffusion: concentration gradient
  2. Thermal diffusion: temperature gradient
  3. Pressure diffusion: pressure gradient
  4. Forced diffusion: unequal external forces on components



Solute transport is from the left to the right; movement of the solutes is due to the concentration gradient (dC/dx).

Q1. Give example(s) for mass transfer based on each of the above driving forces

Fick's 1st Law of Diffusion

Flux of component A in the x direction

$$J_{A,x} = \frac{dn_A}{dt}\frac{1}{A} = -D_{AB}\frac{dc_A}{dx}$$

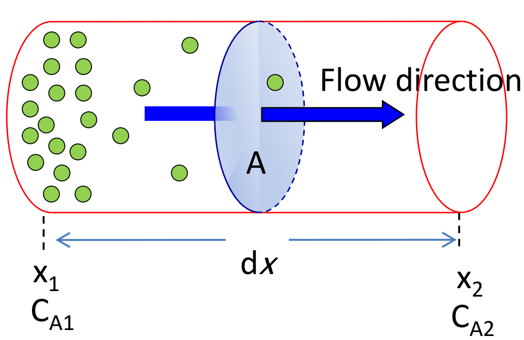
Diffusion coefficient (diffusivity) of component A in B

No. of atoms crossing area A per unit time

Concentration gradient

Cross-sectional area

Matter transport is down the concentration gradient



Note 1

- Mass transfer occurs by two basic mechanisms:
  (1) *molecular diffusion by random and spontaneous* ***microscopic*** **movement** of individual molecules in a gas, liquid, or solid as a result of thermal motion; and
  (2) *eddy (turbulent) diffusion by random,* ***macroscopic*** *fluid motion.*
- *Both* molecular and/or eddy diffusion frequently involve the movement of different species in opposing directions.
- When a net flow occurs in one of these directions, the total rate of mass transfer of individual species is increased or decreased by **this bulk flow** or ***convection effect, which may be*** **considered a third mechanism of mass transfer.**
- Molecular diffusion is extremely slow, whereas eddy diffusion is orders of magnitude more rapid.

Note 2

- Molecular diffusion occurs in solids and in fluids that are stagnant or in laminar or turbulent motion.
- Eddy diffusion occurs in fluids in turbulent motion.
- When both molecular diffusion and eddy diffusion occur, they take place in parallel and are additive.
- Both of them take place because of the same concentration difference (gradient).

Note 3 _ eddy diffusivity term 'ε'

For turbulent momentum transfer and constant density,

$$\tau_{zx} = -\left(\frac{\mu}{\rho} + \varepsilon_t\right)\frac{d(v_x \rho)}{dz}$$

For turbulent heat transfer for constant ρ and c_p,

$$\frac{q_z}{A} = -(\alpha + \alpha_t)\frac{d(\rho c_p T)}{dz}$$

For turbulent mass transfer for constant c,

$$J^*_{Az} = -(D_{AB} + \varepsilon_M)\frac{dc_A}{dz}$$

In these equations ε_t is the turbulent or eddy momentum diffusivity in m^2/s, α_t the turbulent or eddy thermal diffusivity in m^2/s, and ε_M the turbulent or eddy mass diffusivity in m^2/s.

See Geankoplis

Note _ 4
Flux Fick's law

$$J_{A,z} = -D_{AB}\frac{dc_A}{dz}$$

where $J_{A,z}$ is the molar flux in the z direction relative to the molar-average velocity, dc_A/dz is the concentration gradient in the z direction, and D_{AB}, the proportionality factor, is the *mass diffusivity* or *diffusion coefficient* for component A diffusing through component B.

$$\mathbf{J}_A = -D_{AB}\nabla c_A$$

Question : Explain the above equation

$$\text{flux} = -\begin{pmatrix}\text{overall}\\ \text{density}\end{pmatrix}\begin{pmatrix}\text{diffusion}\\ \text{coefficient}\end{pmatrix}\begin{pmatrix}\text{concentration}\\ \text{gradient}\end{pmatrix}$$

$$J_{A,z} = -cD_{AB}\frac{dy_A}{dz}$$

Molar Flux

$$j_{A,z} = -\rho D_{AB}\frac{d\omega_A}{dz}$$

Mass Flux

Question : verify the above two equations.