Principles of Chemical Engineering

Mass Transfer

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Syllabus Contents

Mass transfer operation
Diffusion

Objectives

- To introduce the term “Mass Transfer”.
- To give an overview of diffusion.
- To give an overview about mass transfer coefficient.

Introduction to Mass Transfer

- Mass transfer is the study of the transfer of a component in a homogeneous mixture from one phase to another coexisting phase, or within the same phase from a region of high concentration to low concentration.
- Transfer of a component from one phase to the another is due to the difference of chemical potential (μ) of a component in the coexisting phases.
- The direction of mass transfer is from higher chemical potential to lower chemical potential. If $\mu_i^\alpha > \mu_i^\beta$, component i transfers from α to β phase.
- Chemical potential (μ) is a conceptual property. It can be expressed in terms of measurable properties such as mole fraction, concentration, pressure, vapor pressure etc.

Introduction to Mass Transfer (contd..)

- Phase equilibrium (same T and P for the coexisting phases) determines an upper limit for mass transfer. At equilibrium, the chemical potential of a component is same in both the coexisting phases.

  $$\mu_i^{\alpha} = \mu_i^{\beta}$$

  For vapor-liquid equilibrium of ideal solutions,

  $$y_i P = x_i P_i^{\mathrm{sat}} \qquad \text{Raoult's law}$$

  In a simpler way, equilibrium relationship can be expressed as

  $$y_i = m x_i$$

Importance of Mass Transfer

- Mass transfer operations are directed towards separating a substance into its component parts.
  - For mixtures, such separations may be entirely mechanical, e.g. the filtrations of a solid from a suspension in a liquid, or the separation of particles of a solid mixture according to their density. These aspects are covered in Mechanical Unit Operations (or, simply Mechanical Operations).
  - On the other hand, if the operations involve changes in composition of solutions, they are known as Mass Transfer operations.

Introduction to Mass Transfer (contd..)

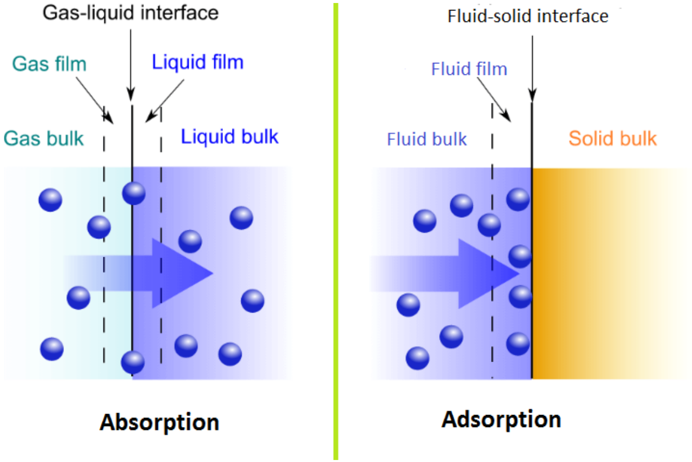
- The importance of mass-transfer operations in chemical engineering is profound. There is scarcely any chemical process which does not require either a preliminary purification of raw materials or a final separation of products from by-products, and for these, mass-transfer operations are commonly used. Frequently, the separations constitute a major part of the costs of a process.

- Examples for Mass Transfer Operations: Absorption, Adsorption, Distillation, Extraction, Leaching, Humidification, Drying.

Examples for Mass Transfer Operations

- **Absorption**: removal of H_2S from natural gas by absorption with monoethanolamine or diethanolamine solutions.
- **Stripping**: removal of oxygen from water (for use with electronic material processing) by contacting with a nitrogen gas.
- **Distillation**: (i) separation of benzene and toluene from a solution of benzene-toluene, (ii) fractionation of petroleum crude oil.
- **Extraction**: (i) removal of adipic acid from water using diethyl ether, (i) removal of mercaptants from naphtha by NaOH solution.
- **Adsorption**: (i) removal of odor / color from materials, using activated carbon, (ii) removal of moisture from air using silica.

Absorption - Adsorption



Absorption of solutes happens in the bulk of the liquid. Adsorption of solutes happens on the surface of the solid.

Mass Transfer Rate

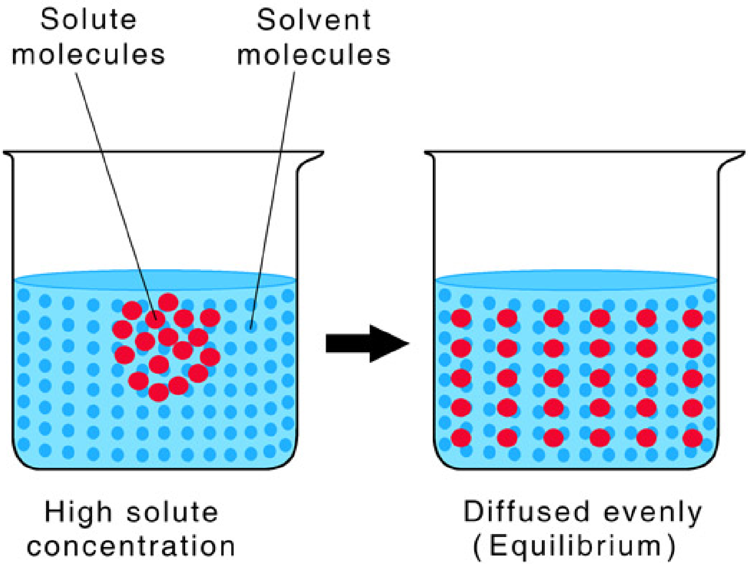
$$N_A = k\Delta C_A = k(C_A - C_A^*)$$

where

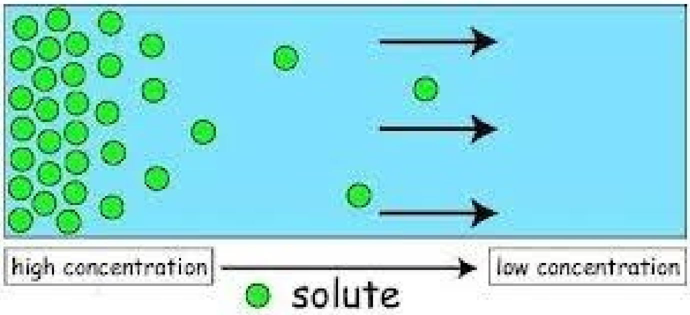
N_A	$=$	mass transfer flux of component A, mol/(area.time)
k	$=$	mass transfer coefficient
C_A	$=$	bulk concentration of A
C_A^*	$=$	equilibrium concentration of A

There are various forms of concentration measures, such as mol/ltr, partial pressure, mole fraction, mole ratio, etc.

Diffusion


Solute molecules
Solvent molecules
High solute concentration
Diffused evenly (Equilibrium)

Diffusion



Diffusion is the process by which molecules, ions, or other small particles spontaneously mix, moving from regions of relatively high concentration into regions of lower concentration.

The molar flux (mol/area.time) due to diffusion of a constituent A relative to the average velocity of all constituents, is given by Fick's first law as

$$\text{Molar flux} = -D_{AB}\frac{\partial C_A}{\partial z}$$

$$\begin{aligned} D_{AB} &= \text{diffusivity or diffusion coefficient of component } A \text{ in } B \\ C_A &= \text{concentration of } A \\ z &= \text{distance} \end{aligned}$$

Fick's first law is applicable to steady state system.

Diffusion

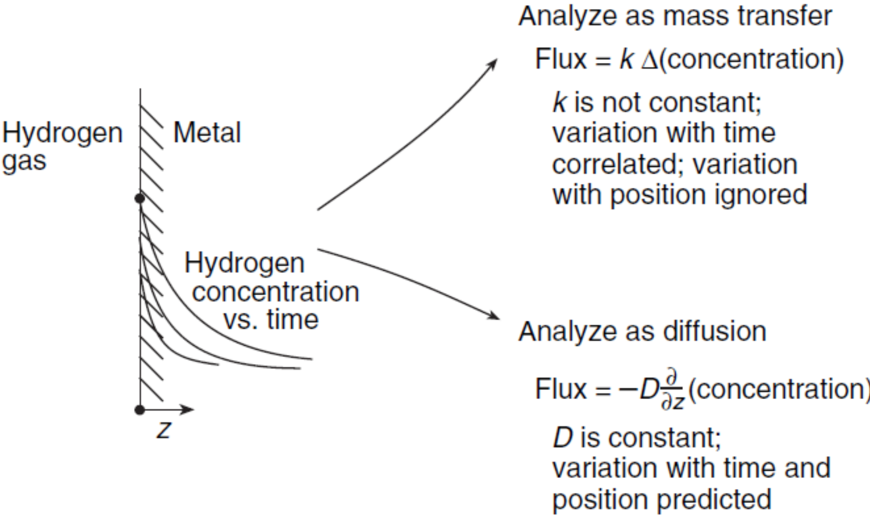
Fick's second law

$$\frac{\partial C_A}{\partial t} = D_{AB}\frac{\partial^2 C_A}{\partial z^2}$$

This describes the transient diffusion phenomenon.

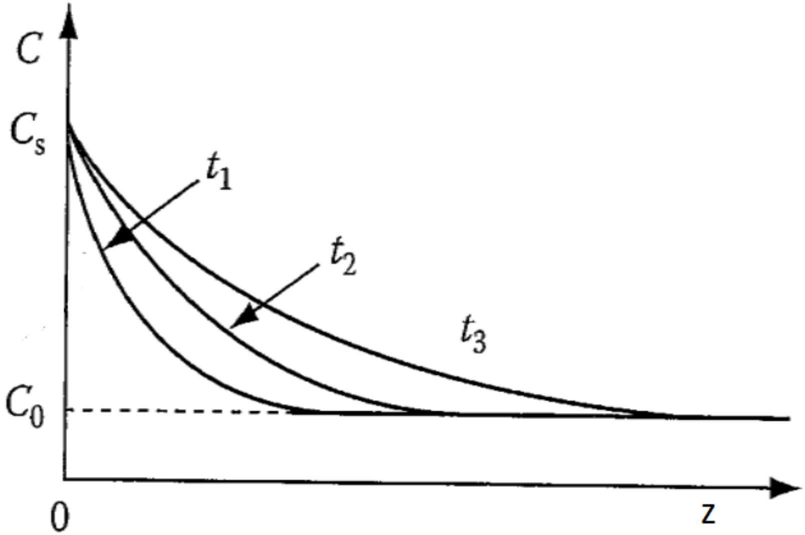
This tells us that rate of change of concentration at a specific time and position is proportional to the second derivative of concentration profile.

Diffusivity and Mass Transfer Coefficient



Ref: Cussler E.L., Diffusion, Cambridge Univ. Press

Diffusivity and Mass Transfer Coefficient (contd..)



Diffusivity and Mass Transfer Coefficient (contd..)

Hydrogen diffusion into a metal: This process can be described with either a mass transfer coefficient (k), or a diffusion coefficient (D_{AB}).

- The description with a diffusion coefficient correctly predicts the variation of concentration with position and time, and so is superior.
- Whereas, the description with mass transfer coefficient predicts the variation, only with time.

Mass Transfer Models based on Diffusivity and Mass Transfer Coefficient

The model based on the diffusion coefficient gives results of more fundamental value than the model based on mass transfer coefficients. In mathematical terms, the diffusion model is said to have distributed parameters, for the dependent variable (the concentration) is allowed to vary with all independent variables (like position and time). In contrast, the mass transfer model is said to have lumped parameters (like the average concentration in the metal).

The diffusion model is more fundamental and is appropriate when concentrations are measured or needed versus both position and time. The mass transfer model is simpler and more approximate and is especially useful when only average concentrations are involved.

Diffusion Coefficient

- Diffusion coefficients in gases lie between 0.1 and 1 cm^2/s.
  - $D_{O_2-He} = 0.822\ cm^2/s$
  - $D_{O_2-\text{benzene}} = 0.101\ cm^2/s$
- Diffusion coefficients in liquid fall close to $10^{-5}\ cm^2/s$. Diffusion coefficients in liquids are about ten thousand times slower than those in dilute gases.
  - $D_{H_2-\text{water}} = 4.5 \times 10^{-5}\ cm^2/s$
  - $D_{\text{acetone}-\text{water}} = 1.21 \times 10^{-5}\ cm^2/s$
  - $D_{\text{ethanol}-\text{water}} = 0.84 \times 10^{-5}\ cm^2/s$
- Diffusion coefficients in solids will be lower than in liquids, about $10^{-30}\ cm^2/s$.
  - $D_{H_2-Fe} = 2 \times 10^{-9}\ cm^2/s$
  - $D_{C-Fe} = 6 \times 10^{-21}\ cm^2/s$
  - $D_{Zn-Cu} = 2 \times 10^{-38}\ cm^2/s$

Diffusion Coefficient (contd..)

- Diffusion coefficients in polymer and glasses lie between solid and liquid values, say about 10^{-8} cm^2/s.
- The low values of diffusion coefficient means that diffusion often limits the overall rate of processes occurring in liquids. Diffusion limits the rate of acid-base reactions. In physiology, diffusion limits the rates of digestion.

Quiz

1. Define ‘mass transfer’.
2. What is the driving force for mass transfer?
3. Give examples for mass transfer operations.
4. Compare between ‘absorption’ and ‘adsorption’.
5. Write the equation for mass transfer flux in terms of diffusivity.
6. Write the equation for mass transfer flux in terms of mass transfer coefficient.
7. Compare between ‘diffusivity model’ and ‘mass transfer coefficient model’ of predicting mass transfer flux.
8. Compare the rate of diffusion of a species in gas, liquid and solid phases.