

Lecture #1

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# **Background:**

PhD Chemical & Biochemical Engineering, University of Iowa, IA, United States, 2022 MSc Chemical Engineering, University of Technology, Iraq, 2012 BSc Chemical Engineering, University of Technology, Iraq, 2006

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# **Course Objectives**

- 1- Understand the basics of diffusion.
- 2- Estimate Molar fluxes in convective and inter-phase mass transfer.
- 3- Explain the concept of diffusion theories.
- 4- Learn how to calculate mass transfer rates in multiple unit operations.





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#### Resources

- Coulson, J. M & Richardson J. F. (2006). "Chemical engineering, Volume 1",
   3P rdP Edition, Robert Maxwell. M. C.
- Dutta Binary K. (2007), "Principles of Mass Transfer & Separation Process", Bvt. Ltd. Prentice Hall, ISPN 8-1203-2990-2.
- Treybal Robert E. (1975), "Mass transfer Operation" 2ed Edition, Mc-Graw-Hill Book.
- McCabe, W., Smith, J., Harriott, P. (2004), "Unit Operations of Chemical Engineering", M Graw-Hill Co., 7P thP Edition, ISBN0072848235.



## **Topics**

- Definitions
- Diffusion in binary gaseous
- Diffusion in multi-component mixtures
- Diffusion in liquids
- Diffusion in solids
- Diffusion theories
- Diffusion resistances
- Unsteady state mass transfer





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### **Definitions**

# **Chemical Engineering**

Is a discipline of engineering that deals with transforming raw materials into products employing a variety of <u>processes</u> (unit operations), including fluid mechanics, heat transfer, <u>mass transfer</u>, and others.

# **Chemical Engineers**

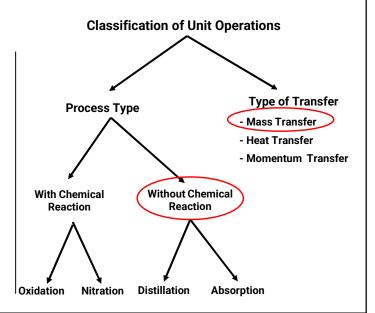
Develop, design, and operate chemical manufacturing processes. Chemical engineers use the principles of chemistry, physics, and engineering to design equipment and **unit operations** for manufacturing products.



## **Definitions**

## **Unit Operations**

The physical operation for manufacturing chemicals deals mainly with the transfer and change of materials and energy principles by physical and physical-chemical means such as **mass**, heat, and momentum transfer





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### **Definitions**

**Mass Transfer** is the movement of molecules or atoms from one location to another, driven by a concentration difference. It occurs in processes like **diffusion**, evaporation, and absorption, and is essential in many chemical engineering operations where substances need to be separated or mixed.

Rate of Transfer process 
$$\alpha$$
  $\frac{\textit{Driving Force}}{\textit{Resistance}}$  ............ General

$$\mathcal{T}=-\,\eta\,rac{du}{dz}$$
  $Newton's~Law$  Momentum Transfer

$$J_A = -D_{AB} rac{dC_A}{dz}$$
 $Fick's\ Law$ 
Mass Transfer

$$q = -krac{dT}{dz}$$
Fourier's Law
Heat Transfer



## **Important Laws**

## 1- Ideal gas law (Boyle's law)

$$PV = nRT$$

R = gas constant

$$=8314 \frac{m^3. p_a}{Kmol. K}$$

$$= 0.082 \frac{m^3. atm}{Kmol. K}$$

$$\frac{P_1 . V_1}{T_1} = \frac{P_2 . V_2}{T_2}$$

### 2- Ideal Gas Mixture (Dalton's law)

$$P_t = P_1 + P_2 + P_3 + \dots = \sum P_i$$

 $P_t$  = Total Pressure

 $P_i$  = Partial Pressure of component (i)

$$P_i = P_t \cdot y_i$$

 $y_i$  = Mole fraction of component (i)

#### 3- Ideal Liquid (Rault's law)

$$P_i = P_i^{\circ} \cdot x_i$$

 $P_i$  = Partial Pressure of component (i)

 $P_i^{\circ}$  = Vapor Pressure of component (i)

 $x_i$ = Mole fraction of component (i) in liquid phase

#### 4- Non – Ideal Mixture (Henry's law)

$$P_i = H. x_i$$

H= Henry's Constant

#### 5- Equilbirium Constant

$$y_i = K_i \cdot x_i$$

### 6- Relative Volatility $\alpha_{AB}$

$$\alpha_{AB} = \frac{\kappa_A}{\kappa_B} = \frac{y_A/x_A}{y_B/x_B} = \frac{p_A^{\circ}}{p_B^{\circ}}$$



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# Concentration, Velocity and Flux

#### 1- Concentratoin expressed as:

$$\rho_i = Mass\ concentration\ of\ i\ \left(\frac{Kg}{m^3}\right)$$

$$ho_t = Total \ mass \ concentration \left( rac{ ext{K}g}{m^3} 
ight) = \sum 
ho_i \ .y_i$$

$$\omega_i = \left(\frac{\rho_i}{\rho_t}\right)$$
 Mass fraction;  $\sum \omega_i = 1$ 

$$C_i = Molar \ concentration \ of \ i \ \left(\frac{Kmol}{2}\right)$$

$$\begin{array}{l} C_i \ = \ Molar \ concentration \ of \ i \ \left(\frac{Kmol}{m^3}\right) \\ C_t \ = \ Total \ molar \ concentration \ \left(\frac{Kmol}{m^3}\right) = \ \sum C_i \ . \ X_i \end{array}$$

$$X_i = \left(\frac{C_i}{C_t}\right)$$
 Mole fraction;  $\sum X_i = 1$ 

#### **Note**

- Gas mole fraction is expressed  $y_i = \left(\frac{P_i}{P_a}\right)$
- Liquid mole fraction is expressed  $X_i = \left(\frac{C_i}{C_r}\right)$

# 2- Average velocity expressed as:

Mass average velocity 
$$u = \left(\frac{1}{\rho_t}\right) \cdot \sum \rho_i \cdot u_i$$

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

#### 3- Flux is expresed as

Flux is a measure of the quantity of material (mass, moles, or volume) moves through a given area per unit time.

 $\label{eq:matter} \textbf{Mathematically Flux} = \frac{Amount\ of\ substance\ transferred}{}$ 

- Mass flux expressed in  $(\frac{Kg}{m^2.Sec})$
- Molar flux expressed in  $\left(\frac{Kmol}{m^2.Sec^2}\right)$



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## Example (1)

A gas mixture ( $N_2 = 5\%$ ,  $H_2 = 15\%$ ,  $NH_3 = 76\%$  and Ar = 4%) flows through a pipe of 25.4 mm in diameter at 4.05 bar total pressure. If the velocities of the components are 0.03, 0.035, 0.03, and 0.02 m/s, respectively.

Calculate: Mass avg., Molar avg., and Volume avg. velocities of the mixture?

Given that: Mwt for N<sub>2</sub> =28, NH<sub>3</sub> = 17, Ar = 40  $(\frac{Kg}{Kmol})$ 

#### Solution

- Mass avg. velocity 
$$u = \left(\frac{1}{\rho_t}\right)$$
.  $\sum \rho_i \cdot u_i$  ;

; 
$$ho_i = rac{P_i \cdot Mwt_i}{R \cdot T}$$
 ;  $ho_t = rac{P_t \cdot Mwt_t}{R \cdot T}$ 

$$u = \frac{R.T}{P_t.Mwt_t} \left( \frac{P_1.Mwt_1}{R.T} \cdot u_1 + \frac{P_2.Mwt_2}{R.T} \cdot u_2 + \frac{P_3.Mwt_3}{R.T} \cdot u_3 + \frac{P_4.Mwt_4}{R.T} \cdot u_4 \right)$$
 ;  $y_i = \left( \frac{P_i}{P_t} \right)$ 

$$u = \frac{1}{Mwt_t} (y_1.Mwt_1.u_1 + y_2.Mwt_2.u_2 + y_3.Mwt_3.u_3 + y_4.Mwt_4.u_4)$$
 ;  $Mwt_t = \sum y_i.Mwt_i$ 

$$Mwt_t = y_1 . Mwt_1 + y_2 . Mwt_2 + y_3 . Mwt_3 + y_4 . Mwt_4$$

$$= 0.05 \times 28 + 0.15 \times 2 + 0.76 \times 17 + 0.04 \times 40 \qquad \rightarrow \quad Mwt_t = 16.22 \frac{\kappa g}{\kappa mol}$$
 
$$u = \frac{1}{16.22} (0.05 \times 28 \times 0.03 + 0.15 \times 2 \times 0.035 + 0.76 \times 17 \times 0.03 + 0.04 \times 4 \times 0.02) \quad \rightarrow \quad u = 0.029 \; \text{m/sec.}$$



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# Example (1)

#### Solution

- Molar avg. velocity  $U = \left(\frac{1}{C_t}\right) \cdot \sum C_i \cdot u_i$  $= \frac{1}{C_t} (C_1 \cdot u_1 + C_2 \cdot u_2 + C_3 \cdot u_3 + C_4 \cdot u_4)$  $y_i = x_i = \left(\frac{c_i}{c_t}\right)$ For gases

$$y_i = x_i = \left(\frac{1}{c_t}\right)$$

$$U$$
= 0.05 \* 0.03 + 0.15 \* 0.035 + 0.76 \* 0.03 + 0.04 \* 0.02  $U$ = 0.0303 m/sec

- Volume avg. velocity

For gases (Volume avg. velocity = Molar avg. velocity)

## <u>H.W. 1</u> Prove that

$$U_t = x_a.u_a + x_b.u_b$$



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