

DETERMINATION OF GAS DIFFUSION COEFFICIENT

Objective:

The objective of this experiment is to calculate diffusion coefficient of a volatile organic compound in air by means of Chapman Enskog equation at room condition.

Background:

The basic unit operations in engineering are momentum, heat and mass transfer. Momentum transfer can be observed in fluid flowing, mixing, and precipitation or filtration operations. Heat transfer in the form of conductive or convective can be seen in evaporation distillation and drying processes. Distillation, absorption, drying, liquid-liquid extraction, adsorption and membran operations are generally utilized from mass transfer equations in order to model and design of a unit under optimum dimensions and operations conditions.

Properties of materials used in physical, chemical or biological processes are very important. Therefore, the properties of the fluids are the key elements in proses design and engineering applications. Diffusion coefficient is among the most important properties of the fluids. When there is a concentration difference in a stagnant fluid, mass transfer can be described by a diffusion. When a droplet of ink drops into a glass of full of water, the blue color of ink is dispersed gradually in water and at the end, obtained a uniform mixture is a known fact. Similar behavior can be observed for gases. Mass transfer is occurred from high concentration to low concentration. Concentration can be defined as mass or molar units. Mass flux ($\text{kg}/\text{m}^2.\text{s}$) is the amount of mass transferred per unit time and per unit area, molar flux ($\text{kmol}/\text{m}^2.\text{s}$) is defined as the transfer of a compound in its molar quantity per unit time and per unit area.

Diffusional flux is proportional to the concentration gradient of a substance and the proportionality constant is defined as a diffusion coefficient. This can be explained by Fick's first law. For a system of binary components, if diffusion of A in B is shown as D_{AB} , Fick's first law can be written for component A;

$$J_A = -cD_{AB} \frac{dx_A}{dz} \quad (1)$$

where, J_A is the diffusional flux of molecule A in the z direction (mol/cm^2), c is concentration (mol/cm^3) and dx_A/dz is the change in mole fraction of A with respect to z direction ($1/\text{m}$). Using

the corresponding units in Equation 1 and taking the unit time as second, the unit of diffusion coefficient is estimated as cm^2/s . The minus sign in Equation 1 reflects that the mass transfer is occurred in the direction of reducing concentration. Equation 1 can only be used if there is no bulk flow. In the case of bulk motion, its contribution to the total flux of i can be represented as follows;

$$N_i = x_i \sum_{j=1}^n N_j + J_i \quad (2)$$

By using Equation 2 for a binary system, total flux of component A relative to a stationary reference point can be defined in terms of molar quantities by the expression given below [1];

$$N_A = (N_A + N_B)x_A - cD_{AB} \frac{dx_A}{dz} \quad (3)$$

Examples of Mass Transfer Processes

Mass transfer is important in many areas of engineering and science. Mass transfer occurs when a component in a mixture migrates in the same phase or from phase to phase because of a difference in concentration between two points. Liquid in an open pail of water evaporates into still air because of the difference in concentration of water vapor at the water surface and surrounding air. There is a driving force from the surface to the air. In a fermentation process nutrients and oxygen dissolved in the solution diffuse to the microorganisms. In a catalytic reaction the reactants diffuse from the surrounding medium to the catalyst surface, where reaction occurs. Distillation of ethanol in water is another example of mass transfer [2].

Special Case for A Diffusing Through Stagnant, Nondiffusing B

In the case of diffusion of A through stagnant or nondiffusing B at steady-state, it is assumed that one boundary at the end of the diffusion path is impermeable to component B, so it cannot pass through. One example, shown in Figure 1, is in the evaporation of a pure liquid such as acetone (A) at the bottom of narrow tube, where a large amount of inert or nondiffusing air (B) is passed over the top. The boundary at the liquid surface at point 1 is impermeable to air, since air is insoluble in acetone liquid. At point 2 the partial pressure $p_{A2}=0$, since a large amount of air is passing by.

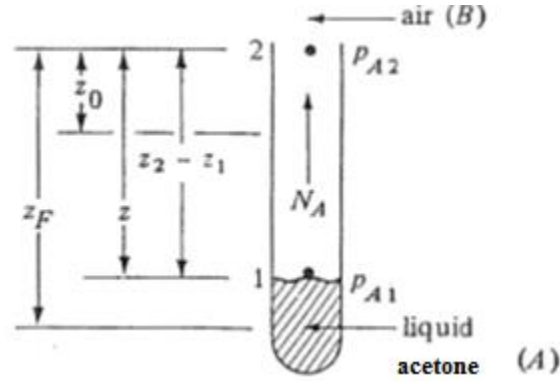


Figure 1: Diffusion of A through stagnant, nondiffusing B

To derive the case for A diffusing in stagnant, nondiffusing B, $N_B=0$ is substituted into the general Equation (3).

$$N_A = -cD_{AB} \frac{dx_A}{dz} + \frac{c_A}{c} (N_A + 0) \quad (4)$$

Keeping the total pressure constant, substituting $c=P/RT$, $p_A=x_AP$, and $c_A/c=p_A/P$ into Equation (4) gives,

$$N_A = -\frac{D_{AB}}{RT} \frac{dp_A}{dz} + \frac{p_A}{P} N_A \quad (5)$$

Rearranging and integrating,

$$N_A \int_{z_1}^{z_2} dz = -\frac{D_{AB}}{RT} \int_{p_{A1}}^{p_{A2}} \frac{dp_A}{1 - p_A/P} \quad (6)$$

$$N_A = \frac{D_{AB}P}{RT(z_2 - z_1)} \ln \frac{P - p_{A2}}{P - p_{A1}} \quad (7)$$

Equation (7) is the final equation to be used to calculate the flux of A. However, it is often written in another form. A log mean value of the inert B is defined as follows. Since $P = p_{A1} + p_{B1} = p_{A2} + p_{B2}$,

$$p_{BM} = \frac{p_{B2} - p_{B1}}{\ln(p_{B2}/p_{B1})} = \frac{p_{A1} - p_{A2}}{\ln[(P - p_{A2})/(P - p_{A1})]} \quad (8)$$

Substituting Equation (8) into Equation (9),

$$N_A = \frac{D_{AB}P}{RT(z_2 - z_1)p_{BM}} (p_{A1} - p_{A2}) \quad (9)$$

Diffusion in a Tube with Change in Path Length

At a given time t , the level z from the top drops slowly as diffusion proceeds (Figure 1). The change in liquid level in a narrow tube can be derived by using the initial and final conditions of the liquid level. Pseudo-steady-state condition can be assumed since, level drops slowly. As time progresses, the path length z increases. Assuming a cross sectional area of 1 m^2 , the level drops dz (m) in dt (s) and $\rho_A(dz \cdot 1)/M_A$ (kmol of A that have left and diffused). Then,

$$N_A \cdot 1 = \frac{\rho_A(dz \cdot 1)}{M_A dt} \quad (10)$$

At any time t , Equation (9) holds; but the path length is z and Equation (9) becomes as follows, where N_A and z are now variables:

$$\frac{\rho_A}{M_A} \int_{z_0}^{z_F} z dz = \frac{D_{AB} P(p_{A1} - p_{A2})}{RT p_{BM}} \int_0^{t_F} dt \quad (11)$$

Solving for t_F ,

$$t_F = \frac{\rho_A (z_F^2 - z_0^2) RT p_{BM}}{2 M_A D_{AB} P(p_{A1} - p_{A2})} \quad (12)$$

Experimental Set-up

The experimental set-up is comprised of a test tube with an internal diameter of 6 mm, measuring cylinder whose hold up volume is 25 mL, a pump for air flowing and analytical balance for taring the mass change.

Running the Experimental Set-up

1. Put acetone into test tube up to 4 mL
2. Record the initial amount of the acetone.
3. Air is flowing above the test tube by means of a pump at a constant flowrate.
4. Record the mass of acetone at each 15 minutes.

References

1. Geankoplis, C.J., Transport Processes-Momentum, Heat, Allyn and Bacon, Boston, (1983).
2. McCabe W.L., Smith J., Harriot P., Unit operations of Chemical Engineering, McGraw Hill International Editions, 5th ed., Singapore (1993).

Data that will be recorded

Time (s)	Mass (g)

Calculations

- Liquid levels at the end of each data recording.
- After recording the initial z value (z_0), calculate and then record the z value at each time interval utilizing from the mass relation as given below;

$$z_t = \frac{(m_0 - m_t)}{\rho_{AA}} + z_0$$

Time (s)	z_t (m)

According to Equation (12), the slope of time vs square of the change in liquid level is proportional to $1/D_{AB}$. The remaining terms except $1/D_{AB}$ on the right hand side of Equation (12) can be assigned to any x .

Time (s)	x

- Plot x with respect to t , and add the graph below.
- Compare the value of diffusivity you calculated with the values in literature.
- If there is a large difference, define the possible errors in experiments and make suggestion to get better result.

Vapor pressure of acetone at $20^{\circ}\text{C} = 118 \text{ mmHg}$

Density of acetone = 790 kg/m^3

Molecular weight of acetone = 58.08 kg/kmol .