

Diffusion (Question and Answer)

Part A

1. What is meant by molecular diffusion and eddy diffusion?

It is concerned with the movement of individual molecules through a substance by virtue of their thermal energy. The phenomenon of molecular diffusion ultimately leads to a completely uniform concentration of substances throughout the solution which may initially have been non uniform.

(OR)

It is the movement of particle from a region of higher concentration to a region of low concentration Example : a lump of sugar dropped into a cup of water will diffuse by diffusion.

2. Define eddy diffusivity.

Diffusion is not restricted to molecular transfer through stagnant layers of solid or fluid. It also takes place when fluids of different compositions are mixed. The first step in mixing is often mass transfer caused by the eddy motion characteristics of turbulent flow. This is Eddy diffusivity.

(OR)

The mechanical agitation produces rapid movement of relatively large chunk or eddies of fluid characteristic of turbulent motion which carry the solute with them. This method of solute transfer is called eddy or turbulent diffusion.

3. State Fick's first law of diffusion.

The Fick's first law of diffusion can be stated as-

$$J_A = - D_{AB} (\partial C_A / \partial z) \\ = - c \cdot D_{AB} (\partial X_A / \partial z)$$

Where,

J_A = flux in mol/(area)(time)

$\partial C_A / \partial z$ = concentration gradient

D_{AB} = diffusivity or diffusion coefficient in m^2/s , A into B

The diffusivity of a constituent A in solution in B, which is a measure of its diffusive mobility, is defined as the ratio of its flux to its concentration gradient which is the Fick's first law written for the z-direction. The negative sign emphasizes that diffusion occurs in the direction of a drop in concentration.

4. State Fick's second law of diffusion.

$$\partial C_A / \partial \theta = D_{AB} (\partial^2 C_A / \partial x^2 + \partial^2 C_A / \partial y^2 + \partial^2 C_A / \partial z^2)$$

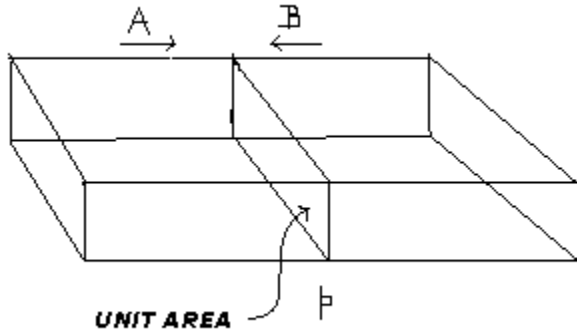
Where

$\partial C_A / \partial \theta$ = Rate of change of concentration, Moles/Area Time

D_{AB} = Diffusivity of 'A' in 'B' - m^2/s

$\partial^2 C_A / \partial x^2$, $\partial^2 C_A / \partial y^2$, $\partial^2 C_A / \partial z^2$ - change of concentration in three directions.

5. For a binary system prove $D_{AB} = D_{BA}$



Consider the element of fluid of unit cross sectional area. To the left of the Section 'P' the concentration of the substance 'A' is higher than the right, while that of 'B' is higher on the right than on the left. Diffusion of the substance then occurs in the directions then shown. the volume rate (or velocity for unit cross section) of movement of 'A' is U_A , that of 'B' is $U_B = -U_A$, and the volume on either side of the section at 'P' remains constant. The rate at which moles of 'A' passes an observer at 'P' is

$$N_A = U_A \rho_A / M_A = U_A C_A$$

And for 'B',

$$N_B = U_B \rho_B / M_B = U_B C_B$$

Where C_A and C_B are the molar concentrations of the constituents. The net rate of movement of moles past the observer at P is $N_A + N_B$,

And the molar average of the velocities is,

$$U_M = (U_A C_A + U_B C_B) / C = (N_A + N_B) / C$$

where C = total molar concentration or density = $C_A + C_B$. The flux N_A with respect to the fixed position 'P' must be larger than ' J_A ' by the amount of 'A' in the volume rate U_M , or

$$N_A = U_M C_A + J_A$$

$$N_A = [(N_A + N_B) C_A / C] - D_{AB} (dC_A / dZ)$$

for 'B',

$$N_B = [(N_A + N_B) C_B / C] - D_{BA} (dC_B / dZ)$$

adding these,

$$-D_{AB} (dC_A / dZ) = D_{BA} (dC_B / dZ)$$

or, $J_A = -J_B$, if $C_A + C_B = \text{constant}$, it follows that $D_{AB} = D_{BA}$ at the prevailing concentration and temperature. thus we have,

$$D_{AB} = D_{BA}$$

7. Write the general equation for the steady state unidirectional molecular diffusion in fluids at rest and in laminar flow

$$N_A = [N_A / (N_A + N_B)] (D_{AB} C / z) \ln \left\{ \frac{[N_A / (N_A + N_B)] - (C_{A2} / C)}{[N_A / (N_A + N_B)] - (C_{A1} / C)} \right\}$$

Where

N_A = Flux of diffusion relative to a fixed surface of component A,

Gmoles/(sec)(sq cm) or lbmoles/(hr)(sq ft)

N_B = Flux of diffusion relative to a fixed surface of component B,

Gmoles/(sec)(sqcm) or lbmoles/(hr)(sqft)

D_{AB} = Diffusivity of component A in Component B,

(sq cm)/sec or sq ft/hr

C = Concentration, (g moles/cu cm) or (lb moles/cu ft)
 Z = distance in the z direction, cm or ft
 C_{A1} = Concentration of component A in point 1
 C_{A2} = Concentration of component A in point 2

8. Write Wilke Chang equation and its uses?

$$D_{AB} = \frac{(117.3 \times 10^{-18}) (\bar{M}_B)^{0.5} T}{\bar{\nu}_A^{0.6}}$$

where,

D_{AB} = Diffusivity of A in very dilute solution in Solvent B m^2/s

\bar{M}_B = Molecular Weight of solvent kg/kg mole

T = Temperature in Kelvin

$\bar{\nu}$ = Solution viscosity kg/m.s

$\bar{\nu}_A$ = Solute molal volume at normal boiling point $m^3/Kmole$

= 0.0756 for water as solute

\bar{O} = Association factor

= 2.26 for water as solvent.

USES:-

This equation can be used for dilute solution of non electrolyte. It is an Empirical equation used to find out diffusivity of liquids.

10. What is the effect of temperature and pressure on the diffusivity of gases?

$$D_{AB} = 10^{-4} (1.084 - 0.249 \sqrt{1/M_A + 1/M_B}) T^{3/2} \sqrt{(1/M_A + 1/M_B) / [P(r_{AB})^2] (KT/\epsilon_{AB})}$$

Where D_{AB} = diffusivity, m^2/hr

T = Absolute temperature, K

M_A, M_B = molecular weight of components A and B respectively Kg/Kmol

P = abs pressure, N/m^2

r_{AB} = molecular separation at collision, mm $(r_A + r_B)/2$

ϵ_{AB} = energy of molecular attraction = $\sqrt{\epsilon_A \epsilon_B}$

$f(kT/\epsilon_{AB})$ = collision function given by graph kT/ϵ Vs $f(kT/\epsilon)$

k = Boltzmann's constant

From this equation it can be seen that the diffusion coefficient is the function of both temperature and pressure.

11. What are the factors that affect the mass transfer rate between two fluids?

Contact area between the two fluids

Hydrodynamic behavior of the flow

Concentration difference between the fluids i.e., of the components

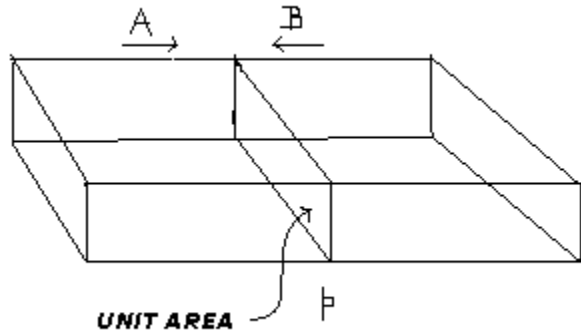
Diffusion property of each component

Pressure

Temperature

Part -B

1. Derive from the first principle the general rate equation for the steady state unidirectional molecular diffusion in fluids at rest and in laminar flow.



Consider the element of fluid of unit cross sectional area. To the left of the Section 'P' the concentration of the substance 'A' is higher than the right, while that of 'B' is higher on the right than on the left. Diffusion of the substance then occurs in the directions then shown. the volume rate (or velocity for unit cross section) of movement of 'A' is U_A , that of 'B' is $U_B = - U_A$, and the volume on either side of the section at 'P' remains constant. The rate at which moles of 'A' passes an observer at 'P' is

$$N_A = U_A \rho_A / M_A = U_A C_A$$

And for 'B',

$$N_B = U_B \rho_B / M_B = U_B C_B$$

Where C_A and C_B are the molar concentrations of the constituents. The net rate of movement of moles past the observer at P is $N_A + N_B$,

And the molar average of the velocities is,

$$U_M = (U_A C_A + U_B C_B) / C = (N_A + N_B) / C$$

where $C =$ total molar concentration or density $= C_A + C_B$. The flux N_A with respect to the fixed position 'P' must be larger than ' J_A ' by the amount of 'A' in the volume rate U_M , or

$$N_A = U_M C_A + J_A$$

$$N_A = [(N_A + N_B) / C] C_A - D_{AB} (dC_A / dz)$$

for 'B', $N_B = [(N_A + N_B) / C] C_B - D_{BA} (dC_B / dz)$

Applying the rate equation to the case of diffusion only in the z direction, with N_A and N_B both constant (steady state), the variables are readily separated, and if D_{AB} is constant, it may be integrated

$$\text{Integ of } [-dC_A / [N_A C - C_A (N_A + N_B)]] \text{ betw } C_{A1} \text{ to } C_{A2} \\ = [1/cD_{AB}] \text{ Integ of } [dz] \text{ betw } Z_1 \text{ to } Z_2$$

Where 1 indicates the beginning of the diffusion path (C_A high), and 2 the end of the diffusion path (C_A low)

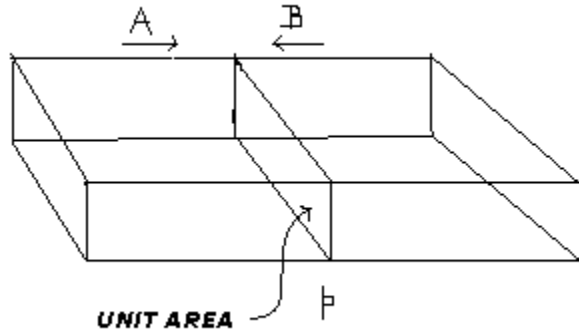
Letting $Z_2 - Z_1 = Z$

$$1/ (N_A + N_B) \ln [(N_A C - C_{A2} (N_A + N_B)) / [(N_A C - C_{A1} (N_A + N_B))] = Z / CD_{AB}$$

$$N_A = [N_A / (N_A + N_B)] (D_{AB} C / Z) \ln [(N_A / (N_A + N_B) - C_{A2} / C) / [(N_A / (N_A + N_B) - C_{A1} / C)]]$$

The above equation is known as steady state molecular diffusion in fluids at rest and in laminar flow.

2. Derive from the first principle the general rate equation for the steady state unidirectional molecular diffusion in gases at rest and in laminar flow.



Consider the element of fluid of unit cross sectional area. To the left of the Section 'P' the concentration of the substance 'A' is higher than the right, while that of 'B' is higher on the right than on the left. Diffusion of the substance then occurs in the directions then shown. The volume rate (or velocity for unit cross section) of movement of 'A' is U_A , that of 'B' is $U_B = -U_A$, and the volume on either side of the section at 'P' remains constant. The rate at which moles of 'A' passes an observer at 'P' is

$$N_A = U_A \rho_A / M_A = U_A C_A$$

And for 'B',
$$N_B = U_B \rho_B / M_B = U_B C_B$$

Where C_A and C_B are the molar concentrations of the constituents. The net rate of movement of moles past the observer at P is $N_A + N_B$,

And the molar average of the velocities is,

$$U_M = (U_A C_A + U_B C_B) / C = (N_A + N_B) / C$$

where C = total molar concentration or density = $C_A + C_B$. The flux N_A with respect to the fixed position 'P' must be larger than ' J_A ' by the amount of 'A' in the volume rate U_M , or

$$N_A = U_M C_A + J_A$$

$$N_A = [(N_A + N_B) / C] C_A - D_{AB} (dC_A / dz)$$

for 'B',
$$N_B = [(N_A + N_B) / C] C_B - D_{BA} (dC_B / dz)$$

Applying the rate equation to the case of diffusion only in the z direction, with N_A and N_B both constant (steady state), the variables are readily separated, and if D_{AB} is constant, it may be integrated

Integration of $[-dC_A / [N_A C - C_A (N_A + N_B)]]$ between C_{A1} to $C_{A2} = [1/cD_{AB}]$ Integ of $[dz]$ betw Z_1 to Z_2

Where 1 indicates the beginning of the diffusion path (C_A high), and 2 the end of the diffusion path (C_A low)

Letting $Z_2 - Z_1 = Z$

$$1/ (N_A + N_B) \ln [(N_A C - C_{A2} (N_A + N_B)) / [(N_A C - C_{A1} (N_A + N_B))] = Z / CD_{AB}$$

$$N_A = [N_A / (N_A + N_B)] (D_{AB} C / z) \ln \{ [N_A / (N_A + N_B)] - (C_{A2} / C) \} / \{ [N_A / (N_A + N_B)] - (C_{A1} / C) \}$$

Where

N_A = Flux of diffusion relative to a fixed surface of component A,
 Gmoles/(sec)(sq cm) or lbmoles/(hr)(sq ft)

N_B = Flux of diffusion relative to a fixed surface of component B,
 Gmoles/(sec)(sqcm) or lbmoles/(hr)(sqft)

D_{AB} = Diffusivity of component A in Component B, (sq cm)/sec or sq ft/hr

C = Concentration, (g moles/cu cm) or (lb moles/cu ft)

Z = distance in the z direction , cm or ft

C_{A1} = Concentration of component A in point 1

C_{A2} = Concentration of component A in point 2

The above equation is known as steady state molecular diffusion in fluids at rest and in laminar flow.

When the ideal gas law can be applied the above equation can be written in a more convenient for use with gases,

Thus , $C_A/C = P_A/P_t = Y_A$

Where P_A = Partial pressure of component 'A'

P_t = Total pressure

Y_A =mole fraction concentration

Further $C = n/v = P_t / R_t$

$$N_A = (N_A / (N_A + N_B)) (D_{AB} P_t / RTZ) \ln [(N_A P_t / (N_A + N_B)) - P_{A2}) / (N_A P_t / (N_A + N_B)) - P_{A1}]$$

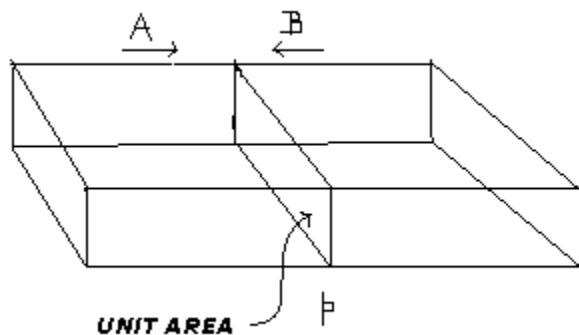
$$N_A = (N_A / (N_A + N_B)) (D_{AB} P_t / RTZ) \ln [(N_A / (N_A + N_B)) - Y_{A2}) / (N_A / (N_A + N_B)) - Y_{A1}]$$

The above equation is known as steady state molecular diffusion in gases at rest and in laminar flow.

3. Derive from the first principle the general rate equation for the steady state unidirectional molecular diffusion in gases at rest and in laminar flow for the following cases.

i). For diffusion of A through non-diffusing B.

ii) For equimolar counter diffusion.



Consider the element of fluid of unit cross sectional area. To the left of the Section 'P' the concentration of the substance 'A' is higher than the right, while that of 'B' is higher on the right than on the left. Diffusion of the substance then occurs in the directions then shown. the volume rate (or velocity for unit cross section) of movement of 'A' is U_A , that of 'B' is $U_B = - U_A$, and the volume on either side of the section at 'P' remains constant. The rate at which moles of 'A' passes an observer at 'P' is

$$N_A = U_A \rho_A / M_A = U_A C_A$$

And for 'B', $N_B = U_B \rho_B / M_B = U_B C_B$

Where C_A and C_B are the molar concentrations of the constituents. The net rate of movement of moles past the observer at P is $N_A + N_B$,

And the molar average of the velocities is,

$$U_M = (U_A C_A + U_B C_B) / C = (N_A + N_B) / C$$

where C = total molar concentration or density = $C_A + C_B$. The flux N_A with respect to the fixed position 'P' must be larger than ' J_A ' by the amount of 'A' in the volume rate U_M , or

$$N_A = U_M C_A + J_A$$

$$N_A = [(N_A + N_B) / C] C_A - D_{AB} (dC_A / dz)$$

for 'B', $N_B = [(N_A + N_B) / C] C_B - D_{BA} (dC_B / dz)$

Applying the rate equation to the case of diffusion only in the z direction, with N_A and N_B both constant (steady state), the variables are readily separated, and if D_{AB} is constant, it may be integrated

Integration of $[-dC_A / (N_A C - C_A (N_A + N_B))]$ between C_{A1} to $C_{A2} = [1/cD_{AB}]$ Integ of $[dz]$ betw Z_1 to Z_2

Where 1 indicates the beginning of the diffusion path (C_A high), and 2 the end of the diffusion path (C_A low)

Letting $Z_2 - Z_1 = Z$

$$1 / (N_A + N_B) \ln [(N_A C - C_{A2} (N_A + N_B)) / (N_A C - C_{A1} (N_A + N_B))] = Z / CD_{AB}$$

$$N_A = [N_A / (N_A + N_B)] (D_{AB} C / z) \ln \{ [N_A / (N_A + N_B)] - (C_{A2} / C) \} / \{ [N_A / (N_A + N_B)] - (C_{A1} / C) \}$$

Where

N_A = Flux of diffusion relative to a fixed surface of component A,

Gmoles/(sec)(sq cm) or lbmoles/(hr)(sq ft)

N_B = Flux of diffusion relative to a fixed surface of component B,

Gmoles/(sec)(sqcm) or lbmoles/(hr)(sqft)

D_{AB} = Diffusivity of component A in Component B,

(sq cm)/sec or sq ft/hr

C = Concentration, (g moles/cu cm) or (lb moles/cu ft)

Z = distance in the z direction, cm or ft

C_{A1} = Concentration of component A in point 1

C_{A2} = Concentration of component A in point 2

The above equation is known as steady state molecular diffusion in fluids at rest and in laminar flow.

When the ideal gas law can be applied the above equation can be written in a more convenient form for use with gases,

Thus, $C_A / C = P_A / P_t = Y_A$

Where P_A = Partial pressure of component 'A'

P_t = Total pressure

Y_A = mole fraction concentration

Further $C = n/v = P_t / R_t$

$$N_A = (N_A / (N_A + N_B)) (D_{AB} P_t / RTZ) \ln [(N_A P_t / (N_A + N_B)) - P_{A2}] / [(N_A P_t / (N_A + N_B)) - P_{A1}]$$

$$N_A = (N_A / (N_A + N_B)) (D_{AB} P_t / RTZ) \ln [(N_A / (N_A + N_B)) - Y_{A2}] / [(N_A / (N_A + N_B)) - Y_{A1}]$$

The above equation is known as steady state molecular diffusion in gases at rest and in laminar flow.

a) Steady state diffusion of A through non-diffusing B.

This might occur, for example, if ammonia (A) were being absorbed from air (B) in to water. In the gas phase, since air does not dissolve appreciably in water, and if we neglect the evaporation of water, only the ammonia diffuses. Thus, $N_B = 0$, $N_A = \text{constant}$,

$N_A / (N_A + N_B) = 1$, substituting in the following equation

$$N_A = \frac{N_A}{(N_A + N_B)} \left(\frac{D_{AB} P_t}{RTZ} \right) \ln \left[\frac{(N_A P_t / (N_A + N_B)) - P_{A2}}{(N_A P_t / (N_A + N_B)) - P_{A1}} \right]$$

$$N_A = \left[\frac{D_{AB} P_t}{RTZ} \right] \ln \left[\frac{(P_t - P_{A2})}{(P_t - P_{A1})} \right]$$

Since $P_t - P_{A2} = P_{B2}$, $P_t - P_{A1} = P_{B1}$, $P_{B2} - P_{B1} = P_{A1} - P_{A2}$

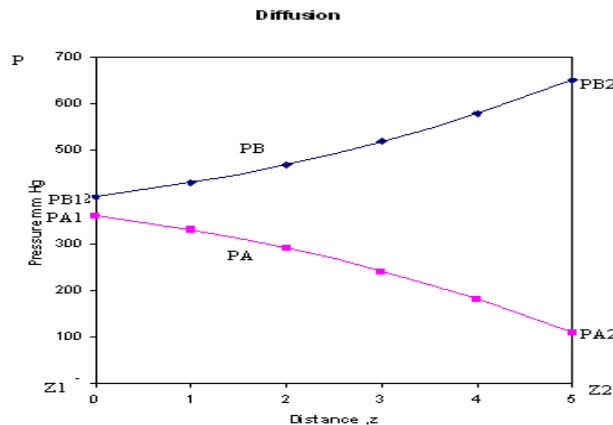
$$N_A = \left[\frac{D_{AB} P_t}{RTZ} \right] \left[\frac{(P_{A1} - P_{A2})}{(P_{B2} - P_{B1})} \right] \ln \left[\frac{(P_{B2})}{(P_{B1})} \right]$$

$$(P_{B2} - P_{B1}) \ln \left[\frac{(P_{B2})}{(P_{B1})} \right] = P_{BM}$$

$$N_A = \left[\frac{D_{AB} P_t (P_{A1} - P_{A2})}{RTZ P_{BM}} \right]$$

This equation is shown graphically

Substance A diffuses by virtue of its concentration gradients, $-dp_A / dz$ Substance B is also diffusing relative to the average molar velocity at a flux J_B which depends upon $-dp_B / dz$, but like a fish which swims upstream at the same velocity as the water flows down stream, $N_B = 0$ relative to a fixed place in space



b. Steady state equimolar counter diffusion.: This is a situation which frequently pertains in distillation operations. $N_A = -N_B = \text{const}$.

$$N_A = \frac{N_A}{(N_A + N_B)} \left(\frac{D_{AB} P_t}{RTZ} \right) \ln \left[\frac{(N_A P_t / (N_A + N_B)) - P_{A2}}{(N_A P_t / (N_A + N_B)) - P_{A1}} \right]$$

The above equation becomes indeterminate, but we can go back to the following equation

$$N_A = \left[\frac{(N_A + N_B)}{C} \right] C_A - D_{AB} \left(\frac{dC_A}{dz} \right)$$

For gases it becomes

$$N_A = (N_A + N_B) \frac{P_A}{P_t} - D_{AB} \frac{dP_A}{RTdz}$$

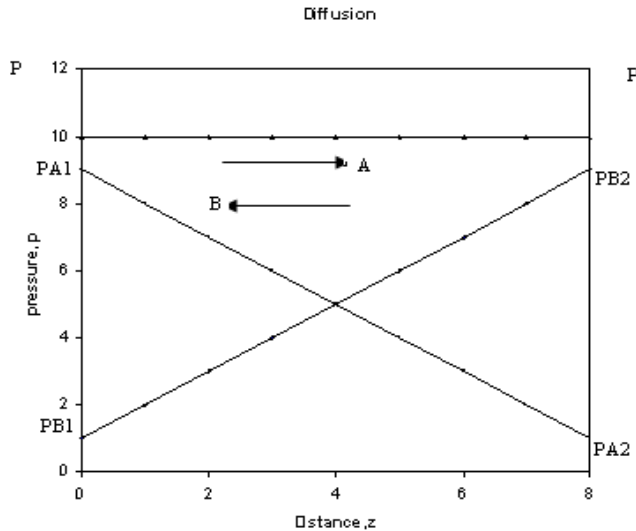
For this case,

$$N_A = - D_{AB} \frac{dP_A}{RTdz}$$

$$\int_{Z_1}^{Z_2} dz = - \frac{D_{AB}}{RTN_A} \int_{P_{A1}}^{P_{A2}} dP_A$$

$$N_A = D_{AB}(P_{A1} - P_{A2}) / RTZ$$

This is shown in graph below



4. Oxygen (A) is diffusing through nondiffusing carbon monoxide (B) under steady state conditions. Total pressure is $1 \times 10^5 \text{ N/m}^2$ and temperature is 0°C . The partial pressure of oxygen (A) at two planes 2mm apart are 13000, 6500 N/m^2 respectively. The diffusivity of the mixture is $1.87 \times 10^{-5} \text{ m}^2/\text{s}$. Calculate the rate of diffusion of oxygen in kmoles per second through each sq.m of the two planes

Formulae to be used :

$$N_A = [D_{AB} P_t / RTZ] \ln [(P_t - P_{A2}) / (P_t - P_{A1})]$$

(OR)

$$N_A = [D_{AB} P_t (P_{A1} - P_{A2})] / RTZ P_{BM}$$

Given Data :

$$D_{AB} = 1.87 \times 10^{-5} \text{ m}^2/\text{s}$$

$$P_t = 101.3 \text{ kPa (} 101.3 \text{ kN/m}^2\text{)}$$

$$P_{A1} = 13 \text{ kN/m}^2$$

$$P_{A2} = 6.5 \text{ kN/m}^2$$

$$R = 8.314 \text{ kJ / kg mole}$$

$$T = 273 \text{ K}$$

$$Z = 2 \times 10^{-3} \text{ m}$$

Calculation :

$$\begin{aligned} N_A &= [D_{AB} P_t \ln [(P_t - P_{A2}) / (P_t - P_{A1})] / RTZ] \\ &= [1.87 \times 10^{-5} \times 101.3 \times \ln [(101.3 - 6.5) / (101.3 - 13)] / (8.314 \times 273 \times 2 \times 10^{-3})] \\ &= [1.87 \times 10^{-5} \times 101.3 / (8.314 \times 273 \times 2 \times 10^{-3})] \times 0.068 \\ &= 2.83 \times 10^{-5} \text{ kgmole/ m}^2\text{s} \end{aligned}$$

(OR)

$$N_A = [D_{AB} P_t (P_{A1} - P_{A2})] / RTZ P_{BM}$$

$$P_t - P_{A2} = P_{B2}, \quad P_t - P_{A1} = P_{B1}, \quad P_{B2} - P_{B1} = P_{A1} - P_{A2}$$

$$P_{B2} = 101.3 - 6.5 = 94.8 \text{ kN/m}^2, \quad P_{B1} = 101.3 - 13 = 88.3 \text{ kN/m}^2$$

$$P_{BM} = (P_{B2} - P_{B1}) / \ln [(P_{B2}) / (P_{B1})]$$

$$P_{BM} = (94.8 - 88.3) / \ln (94.8 / 88.3)$$

$$= 6.5 / 0.068 = 95.6 \text{ kN/m}^2$$

$$N_A = [1.87 \times 10^{-5} \times 101.3 \times (13 - 6.5)] / [8.314 \times 273 \times 2 \times 10^{-3} \times 95.6]$$

$$= 2.84 \times 10^{-5} \text{ kgmole/ m}^2\text{s}$$

5. Methane diffuses at a steady state through a tube containing helium. At a point (1) the partial pressure is 15.55 kpa and at point (2) which is 30 mm apart the partial pressure of methane is 10 kPa. The total pressure is 101.32 kPa and temperature is 293 K. At this pressure and temperature the value of diffusivity is $6.75 \times 10^{-5} \text{ m}^2/\text{sec}$. Calculate the flux of methane at steady state for equimolar counter diffusion.

Formulae to be used :

$$N_A = D_{AB}(P_{A1} - P_{A2}) / RTZ$$

Given Data :

$$D_{AB} = 6.75 \times 10^{-5} \text{ m}^2/\text{sec}$$

$$P_{A1} = 15.55 \text{ kpa}$$

$$P_{A2} = 10 \text{ kPa}$$

$$R = 8.314 \text{ kJ/kg moleK}$$

$$T = 293 \text{ k}$$

$$Z = 30 \text{ mm}$$

Calculation :

$$N_A = D_{AB}(P_{A1} - P_{A2}) / RTZ$$

$$= 6.75 \times 10^{-5} (15.55 - 10) / 8.314 \times 293 \times 30 \times 10^{-3}$$

$$= 5.13 \times 10^{-6} \text{ kgmole/m}^2\text{s}$$

6. In an oxygen – nitrogen gas mixture at 1 atm., 25°C, the concentrations of oxygen at two planes 3 mm apart are 10 and 20 volume % respectively. Calculate the rate of diffusion of oxygen, expressed as kg moles oxygen / m² /sec for the case where there is equimolar counter diffusion of the two gases. The diffusivity for this system is $0.206 \text{ cm}^2 / \text{sec}$

Formulae to be used :

$$N_A = D_{AB}(P_{A1} - P_{A2}) / RTZ$$

Given Data :

$$D_{AB} = 2.06 \times 10^{-5} \text{ m}^2/\text{sec}$$

$$P_{A1} = 0.2 \text{ Pt} = 0.2 \times 1 = 0.2 \text{ atm} = 0.2 \times 101.3 = 20.26 \text{ kN/m}^2$$

$$P_{A2} = 0.1 \text{ Pt} = 0.1 \times 1 = 0.1 \text{ atm.} = 0.1 \times 101.3 = 10.13 \text{ kN/m}^2$$

$$R = 8.314 \text{ kJ/kg mole K}$$

$$T = 273 + 25 = 298 \text{ k}$$

$$Z = 3 \text{ mm}$$

Calculation :

$$N_A = D_{AB}(P_{A1} - P_{A2}) / RTZ$$

$$= 2.06 \times 10^{-5} (20.26 - 10.13) / 8.314 \times 298 \times 3 \times 10^{-3}$$

$$= 2.8 \times 10^{-5} \text{ kgmole/m}^2\text{s}$$

7) What is the rate of diffusion of chloropicrin (CCl_3NO_2) into air at 25°C under the following conditions?

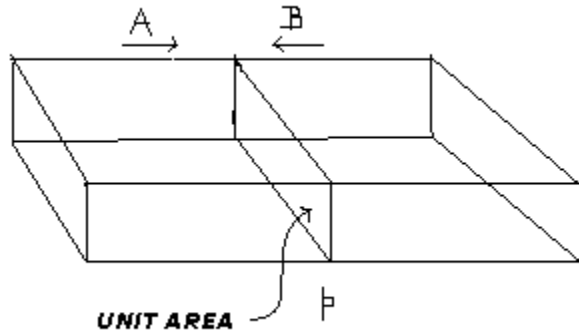
Total pressure = 770 mm Hg

Vapour pressure at 25°C = 23.81 mm Hg

Diffusivity = 0.088 cm²/s
 Length of diffusion path = 11.14 cm.
 Density of chloropicrin = 1.65 g/cm³
 Surface area of liquid exposed = 2.29 cm²

9). Derive from the first principle the general rate equation for the steady state unidirectional molecular diffusion in liquids at rest and in laminar flow for the following cases.

- i) For diffusion of A through non diffusing B.
- ii) For equimolar counter diffusion



Consider the element of fluid of unit cross sectional area. To the left of the Section 'P' the concentration of the substance 'A' is higher than the right, while that of 'B' is higher on the right than on the left. Diffusion of the substance then occurs in the directions then shown. the volume rate (or velocity for unit cross section) of movement of 'A' is U_A , that of 'B' is $U_B = -U_A$, and the volume on either side of the section at 'P' remains constant. The rate at which moles of 'A' passes an observer at 'P' is

$$N_A = U_A \rho_A / M_A = U_A C_A$$

And for 'B', $N_B = U_B \rho_B / M_B = U_B C_B$

Where C_A and C_B are the molar concentrations of the constituents. The net rate of movement of moles past the observer at P is $N_A + N_B$,

And the molar average of the velocities is,

$$U_M = (U_A C_A + U_B C_B) / C = (N_A + N_B) / C$$

where C = total molar concentration or density = $C_A + C_B$. The flux N_A with respect to the fixed position 'P' must be larger than ' J_A ' by the amount of 'A' in the volume rate U_M , or

$$N_A = U_M C_A + J_A$$

$$N_A = [(N_A + N_B) / C] C_A - D_{AB} (dC_A / dz)$$

for 'B', $N_B = [(N_A + N_B) / C] C_B - D_{BA} (dC_B / dz)$

Applying the rate equation to the case of diffusion only in the z direction, with N_A and N_B both constant (steady state), the variables are readily separated, and if D_{AB} is constant, it may be integrated

Integration of $[-dC_A / [N_A C - C_A (N_A + N_B)]]$ between C_{A1} to $C_{A2} = [1/cD_{AB}]$ Integ of $[dz]$ betw Z_1 to Z_2

Where 1 indicates the beginning of the diffusion path (C_A high), and 2 the end of the diffusion path (C_A low)

Letting $Z_2 - Z_1 = Z$

$$1/ (N_A + N_B) \ln [(N_A C - C_{A2} (N_A + N_B)) / [(N_A C - C_{A1} (N_A + N_B))] = Z / CD_{AB}$$

$$N_A = \left[\frac{N_A}{N_A + N_B} \right] \left(\frac{D_{AB} C}{z} \right) \ln \left\{ \frac{\left[\frac{N_A}{N_A + N_B} \right] - \left(\frac{C_{A2}}{C} \right)}{\left[\frac{N_A}{N_A + N_B} \right] - \left(\frac{C_{A1}}{C} \right)} \right\}$$

Where

N_A = Flux of diffusion relative to a fixed surface of component A,
Gmoles/(sec)(sq cm) or lbmoles/(hr)(sq ft)

N_B = Flux of diffusion relative to a fixed surface of component B,
Gmoles/(sec)(sqcm) or lbmoles/(hr)(sqft)

D_{AB} = Diffusivity of component A in Component B,
(sq cm)/sec or sq ft/hr

C = Concentration, (g moles/cu cm) or (lb moles/cu ft)

Z = distance in the z direction , cm or ft

C_{A1} = Concentration of component A in point 1

C_{A2} = Concentration of component A in point 2

The above equation is known as steady state molecular diffusion in fluids at rest and in laminar flow.

Diffusion of A through non diffusing B.

Molecular diffusion in Liquids :

The above equation can be conveniently written as

$$N_A = \frac{N_A}{N_A + N_B} \left(\frac{D_{AB}}{Z} \right) (\rho/M)_{av} \ln \left[\frac{\left(\frac{N_A}{N_A + N_B} \right) - x_{A2}}{\left(\frac{N_A}{N_A + N_B} \right) - x_{A1}} \right]$$

Where ρ and M are the solution density and molecular weight respectively.

x_A indicates mole fraction of component.

Steady state diffusion of 'A' through Non diffusing 'B'

N_A = Constant and $N_B = 0$

$$N_A = \left(\frac{D_{AB}}{Z} \right) (\rho/M)_{av} \ln \left[\frac{(1-x_{A2})}{(1-x_{A1})} \right]$$

Since

$$x_{A1} + x_{B1} = 1$$

$$x_{A2} + x_{B2} = 1$$

$$x_{A1} + x_{B1} = x_{A2} + x_{B2}$$

$$(x_{A1} - x_{A2}) = (x_{B2} - x_{B1})$$

and also

$$1 - x_{A2} = x_{B2}$$

$$1 - x_{A1} = x_{B1}$$

We have

$$N_A = \left(\frac{D_{AB}}{Z} \right) (\rho/M)_{av} \left[\frac{(x_{A1} - x_{A2})}{(x_{B2} - x_{B1})} \right] \ln \left(\frac{x_{B2}}{x_{B1}} \right)$$

$$= \left(\frac{D_{AB}}{Z} \right) (\rho/M)_{av} \left[\frac{(x_{A1} - x_{A2})}{x_{BM}} \right]$$

where $x_{BM} = [(x_{B2} - x_{B1})] \ln (x_{B2}/x_{B1})$

$$N_A = \left(\frac{D_{AB}}{Z} x_{BM} \right) (\rho/M)_{av} (x_{A1} - x_{A2})$$

Steady state Equimolal counter diffusion :

$$N_A = \frac{N_A}{N_A + N_B} \left(\frac{D_{AB}}{Z} \right) (\rho/M)_{av} \ln \left[\frac{\left(\frac{N_A}{N_A + N_B} \right) - x_{A2}}{\left(\frac{N_A}{N_A + N_B} \right) - x_{A1}} \right]$$

$c = (\rho/m)_{avg}$ for liquids

m = molecular weight

ρ = density in kg/m^3

$$N_A = -N_B = \text{Constant}$$

$$N_A = (N_A + N_B) \left(\frac{C_A}{C} \right) - D_{AB} \left(\frac{\partial C_A}{\partial Z} \right)$$

$$\text{Put } N_A = -N_B = \text{Constant}$$

$$N_A = -D_{AB} \left(\frac{\partial C_A}{\partial Z} \right)$$

$$\partial Z = - \left(\frac{D_{AB}}{N_A} \right) \int (\partial C_A)$$

$$Z = (D_{AB}/N_A) * (C_{A1} - C_{A2})$$

$$\text{Put } C_{A1}/C = X_{A1} \text{ and } C_{A2}/C = X_{A2}$$

$$N_A = (D_{AB}/Z) * (\rho/M)_{av} (X_{A1} - X_{A2})$$

10). Calculate the rate of diffusion of Nacl per unit area through a stagnant film of water 1mm thick when the concentration are 9% and 3%(Wt%)respectively oneither side of the film .The diffusivity of Nacl in the solution may be taken as $1.4 \times 10^{-9} \text{ m}^2/\text{sec}$.The density of 9%Nacl at 18°C is 1012 kg/m^3 and 3% solution at 18°C = 1003 kg/m^3

Equations/formula

$$N_A = (D_{AB}/Z X_{BM}) * (\rho/M)_{av} (X_{A1} - X_{A2})$$

$$\text{Where } X_{BM} = (X_{B2} - X_{B1}) / \ln (X_{B2} / X_{B1})$$

$$N_A = (D_{AB}/Z) (\rho/M)_{av} \ln [(1 - X_{A2}) / (1 - X_{A1})]$$

Given :-

Concentration at plane 1=9%(wt%)

Concentration at plane 2=3%(wt%)

$$D_{AB} = 1.4 \times 10^{-9} \text{ m}^2 \text{ sec.}$$

$$\rho_{9\% \text{ Nacl}} = 1012 \text{ kg/m}^3 \text{ at } 18^\circ\text{C}$$

$$\rho_{3\% \text{ Nacl}} = 1003 \text{ kg/m}^3 \text{ at } 18^\circ\text{C}$$

$$Z = 1 \times 10^{-3} \text{ m}$$

9% SOLUTION:-

$$X_{A1} = [(0.09/58)/(0.09/58 + 0.91/18.02)] = 0.0298$$

= 0.0298 mole fraction of Nacl

$$X_{B1} = (1 - X_{A1}) = (1 - 0.0298)$$

= 0.972 mole fraction of water

$$M = 1/(0.09/58) + (0.91/18.02) = 19.21 \text{ kg/kmole}$$

$$\rho/M = 1012/19.21 = 52.7 \text{ kmole/m}^3$$

3% SOLUTION:-

$$X_{A2} = [(0.03/58)/(0.03/58 + 0.97/18.02)] = 0.0095$$

$$X_{B2} = 0.9904 \text{ mole fraction of water}$$

$$M = 1/(0.03/58) + (0.97/18.02) = 18.4 \text{ kg /kmole}$$

$$(\rho/M)_{3\%} = 1003.2/18.4 = 54.52$$

$$(\rho/M)_{av} = [(\rho/M)_{9\%} + (\rho/M)_{3\%}] / 2 = 52.7 + 54.52 / 2 = 53.6$$

= 53.6 kmole/m³

$$X_{Bm} = (X_{B2} - X_{B1}) / \ln [(X_{B2} / X_{B1})]$$

$$= (0.9904 - 0.972) / \ln (0.9904/0.972)$$

= 0.981

$$N_A = (D_{AB}/Z X_{BM}) * (\rho/M)_{av} (X_{A1} - X_{A2})$$

$$= 1.4 \times 10^{-9} \times 53.6 \times (0.0298 - 0.0095) / (1 \times 10^{-3} \times 0.981)$$

= $1.55 \times 10^{-6} \text{ kmole/m}^2 \text{ sec}$

11. Acetic acid is diffusing across a 1 mm thick film of non diffusing water solution. The concentrations on opposite sides of the film are 9 and 3 weight percent acetic acid respectively. The densities of the solutions are 1012 and 1003 kg/m³ respectively. The

diffusivity of acetic acid in solution is $9.5 \times 10^{-8} \text{ m}^2/\text{s}$. Molecular weight of acetic acid is 60 kg/kmol. Determine the diffusion flux of acetic acid.

Solution :

Equation : $N_A = (D_{AB}/Zx_{BM})(\rho/M)_{av} (x_{A1} - x_{A2})$ where $x_{BM} = (x_{B2} - x_{B1}) / \ln (x_{B2}/x_{B1})$

$Z = 0.001\text{m}$, $M_A = 60.03$, $M_B = 18.02$

$x_{A1} = (0.09/60.03) / [(0.09/60.03)+(0.91/18.02)] = 0.0015/0.0520 = 0.0288$ mole fraction of Acetic acid

$x_{B1} = 1 - 0.0288 = 0.9712$ mole fraction of water

$M = 1/0.052 = 19.21 \text{ kg/kmole}$ $(\rho/M) = 1012 / 19.21 = 52.7 \text{ kmole/m}^3$

$x_{A2} = (0.03/60.03) / [(0.03/60.03)+(0.97/18.02)] = 0.0092$ mole fraction of Acetic acid

$x_{B2} = 1 - 0.0092 = 0.9908$ mole fraction of water, $M = 18.4\text{kg/kmole}$

$(\rho/M) = 1003 / 18.4 = 54.5 \text{ kmole/m}^3$ $(\rho/M)_{av} = (52.7+54.5)/2 = 53.6\text{kmol/m}^3$

$x_{BM} = (0.9908 - 0.9712) / \ln(0.9908/0.9712) = 0.98$

$N_A = 9.5 \times 10^{-8} \times 53.6 \times (0.0288 - 0.0092) / (0.001 \times 0.98) = 1.018 \times 10^{-6} \text{ kmol/m}^2\text{s}$

13) Ammonia gas is diffusing at a constant rate through a layer of stagnant air 1 mm thick. Conditions are such that the gas contains 50 per cent by volume ammonia at one boundary of the stagnant layer. The ammonia diffusing to the other boundary is quickly absorbed and the concentration is negligible at that plane. The temperature is 295 K and the pressure atmospheric, and under these conditions the diffusivity of ammonia in air is $1.8 \times 10^{-5} \text{ m}^2/\text{s}$. Estimate the rate of diffusion of ammonia through the layer.

Solution

If the subscripts 1 and 2 refer to the two sides of the stagnant layer and the subscripts A and B refer to ammonia and air respectively, then the rate of diffusion through a stagnant layer is given by:

$N_A = [D_{AB} P_t \ln [(P_t - P_{A2}) / (P_t - P_{A1})] / RTZ]$

(OR) $N_A = [D_{AB} P_t (P_{A1} - P_{A2})] / RTZ P_{BM}$

In this case, $Z = 0.001 \text{ m}$, $D_{AB} = 1.8 \times 10^{-5} \text{ m}^2/\text{s}$, $R = 8314 \text{ J/kmol K}$, $T = 295 \text{ K}$ and $P = 101.3 \text{ kN/m}^2$ and

hence:

$P_{A1} = (0.50 \times 101.3) = 50.65 \text{ kN/m}^2$

$P_{A2} = 0$

$P_{B1} = (101.3 - 50.65) = 50.65 \text{ kN/m}^2 = 5.065 \times 10^4 \text{ N/m}^2$

$P_{B2} = (101.3 - 0) = 101.3 \text{ kN/m}^2 = 1.013 \times 10^5 \text{ N/m}^2$

$P_{BM} = (101.3 - 50.65) / \ln(101.3/50.65) = 73.07 \text{ kN/m}^2 = 7.307 \times 10^4 \text{ N/m}^2$

$P/P_{BM} = (101.3/73.07) = 1.386$.

Thus, substituting in equation :

$N_A = 1.8 \times 10^{-5} / (8314 \times 295 \times 0.001) [1.386(0 - 5.065 \times 10^4)]$

$= 5.15 \times 10^{-4} \text{ kmol/m}^2\text{s}$