- **Molecular Diffusion in fluids :**

  Molecular diffusion, often simply called diffusion, is the thermal motion of all (liquid or gas) particles at temperatures above absolute zero. The rate of this movement is a function of temperature, viscosity of the fluid and the size (mass) of the particles. Diffusion explains the net flux of molecules from a region of higher concentration to one of lower concentration. Once the concentrations are equal the molecules continue to move, but since there is no concentration gradient the process of molecular diffusion has ceased and is instead governed by the process of self diffusion, originating from the random motion of the molecules.

  According to Fick's first law for the z direction

$$J_A = -D_{AB}\frac{dC_A}{dz} = -cD_{AB}\frac{dx_A}{dz}$$

Where J_A = diffusion flux , D_{AB} = diffusion coefficient C_A = concentration gradient

- **Steady-State Molecular Diffusion in Fluids at rest and in Laminar flow:**

  When the diffusion is only in z direction with N_A and N_B both constant we can write the equation

$$\int_{C_{A1}}^{C_{A2}} \frac{-dC_A}{N_A c - C_A(N_A + N_B)} = \frac{1}{cD_{AB}}\int_{z1}^{z2} dz \qquad (1)$$

  Where 1 indicates the beginning of the diffusion path and 2 indicates end of the diffusion path letting $z_2 - z_1 = z$ and integrating we get

$$N_A = \frac{N_A}{N_A + N_B}\frac{D_{AB}c}{z}\ln\frac{N_A/(N_A + N_B) - C_{A2}/c}{N_A/(N_A + N_B) - C_{A1}/c} \qquad (2)$$

- **Molecular Diffusion in gases:**

  When the ideal-gas law can be applied equation (2) can be written in a form more convenient for use with gas. Thus,

$$\frac{C_A}{c} = \frac{P_A}{P_t} = y_A$$

Where P_A = partial pressure of component A

P_t = total pressure Y_A = mole fraction concentration

Further $c = \frac{n}{V} = \frac{P_t}{RT}$

So equation (2) becomes

$$N_A = \frac{N_A}{N_A + N_B}\frac{D_{AB}P_t}{RTz} \ln\frac{[N_A/(N_A + N_B)]P_t - P_{A2}}{[N_A/(N_A + N_B)]P_t - P_{A1}} \qquad (3)$$

Or

$$N_A = \frac{N_A}{N_A + N_B}\frac{D_{AB}P_t}{RTz} \ln\frac{[N_A/(N_A + N_B)]P_t - y_{A2}}{[N_A/(N_A + N_B)]P_t - y_{A1}} \qquad (4)$$

- **Steady-State diffusion of A through non diffusing B:**

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

$$\frac{N_A}{N_A + N_B} = 1$$

  And equation (3) become

$$N_A = \frac{D_{AB}P_t}{RTz} \ln\frac{P_t - P_{A2}}{P_t - P_{A1}} \qquad (4)$$

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

$$N_A = \frac{D_{AB}P_t}{RTz}\frac{P_{A1} - P_{A2}}{P_{B2} - P_{B1}}\ln\frac{P_{B2}}{P_{B1}} \qquad (5)$$

If we let

$$\frac{P_{B2} - P_{B1}}{\ln(P_{B2}/P_{B1})} = P_{B,M}$$

Then

$$N_A = \frac{D_{AB}P_t}{RTzP_{B,M}}\ln(P_{A1} - P_{A2}) \qquad (6)$$

- **Steady-State equimolal counter diffusion:**

This is the situation which frequently pertains in distillation operation. $N_A = -N_B = \text{const}$

Equation (3) becomes indeterminate but we can write according to Ficks law

$$N_A = (N_A + N_B)\frac{P_A}{P_t} - \frac{D_{AB}}{RT}\frac{dP_A}{dz} \qquad (7)$$

Or for this case

$$N_A = -\frac{D_{AB}}{RT}\frac{dP_A}{dz} \qquad (8)$$

$$\int_{z1}^{z2} dz = -\frac{D_{AB}}{RT}\int_{P_{A1}}^{P_{A2}} dP_A \qquad (9)$$

$$N_A = \frac{D_{AB}}{RTz}\ln(P_{A1} - P_{A2}) \qquad (10)$$

- **Molecular Diffusion in liquids:**

  In case of diffusion in liquids , C and D_{AB} may vary considerably with respect to process conditions.

  Hence eq. 2 becomes

$$N_A = \frac{N_A}{N_A + N_B}\frac{D_{AB}}{z}[\frac{\rho}{M}]av \ln\frac{N_A/(N_A + N_B) - C_{A2}/c}{N_A/(N_A + N_B) - C_{A1}/c} \qquad (10)$$

Where ρ is solution density and M is solution molecular weight.

Case-I: Diffusion of liquid A through a stagnant liquid B

$N_B=0$ $N_A=$ Constant.

$$N_A = \frac{D_{AB}}{zX_{B,M}}\left[\frac{\rho}{M}\right] av \ln(X_{A1} - X_{A2}) \qquad (11)$$

Case -II :Equimolal counter diffusion

$N_A= - N_B$

$$N_A = \frac{D_{AB}}{z} * (C_{A1} - C_{A2}) \qquad (12)$$

$$N_A = \frac{D_{AB}}{z}\left[\frac{\rho}{M}\right] av\ (X_{A1} - X_{A2}) \qquad (13)$$

Note: Reference- R.E. Trebal

Assignment (1) : Try to attempt all questions except Q.1,2 and 3, take assumptions if any data is missing