THAPAR INSTITUTE OF ENGINEERING & TECHNOLOGY (Deemed to be University)

Mass Transfer-I

Diffusion (Continue…)

DEPARTMENT OF CHEMICAL ENGINEERING
Thapar Institute of Engineering & Technology
Patiala (Punjab), INDIA-147004

Dr. Avinash Chandra
(Ph.D., IIT Kanpur)
Associate Professor

Web: http://www.thapar.edu/faculties/view/Dr.-Avinash-Chandra/ODU=/Mg==

Relative flux (J_A) *vs* Absolute flux (N_A)

The difference between molecular flux J_A and N_A

- N_A, is the flux of a component 'A' relative to a fixed location in space
- J_A, the flux of component 'A' relative to the average molar velocity of all the constituents

Example:

Imagine a fisherman is fishing in a river with a baited hook. So the fisherman is most interested in the rate at which fish swims upstream against the flowing current to reach his 'baited hook'(the fixed location) is analogous to N_A. Whereas the velocity of fish relative to 'stream' is analogous to J_A which describes the swimming ability of the fish.

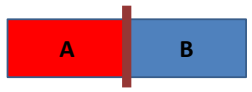
Expression for N_A

Let us consider a box which is divided by two partitions. In left section there is water (A) and in right Section Ethanol (B). Densities of the liquids are different. If we remove the partition, diffusion of both liquid will occur. If the direction to the right is considered positive then flux of A relative to the fixed point is positive and flux of B will be negative. So the Net flux will be $N = N_A + N_B$

The molar average velocity $U = \frac{1}{C}(N_A + N_B)$

Fluxes of A and B are $N_A = C_A u_A$; $N_B = C_B u_B$

$$J_A = -D_{AB}\frac{dC_A}{dz} = C_A(u_A - U)$$
$$= C_A u_A - C_A U$$
$$= N_A - \frac{C_A}{C}(C_A u_A + C_B u_B)$$
$$= N_A - \frac{C_A}{C}(N_A + N_B)$$
$$N_A = (N_A + N_B)\frac{C_A}{C} - D_{AB}\frac{dC_A}{dz}$$



N_A is the molar flux of A in a binary mixture with respect to a stationary observer

The molar flux (N_A) in a stationary frame of reference

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

$(N_A + N_B)\frac{C_A}{C}$ → bulk flow

$D_{AB}\frac{dC_A}{dz}$ → Molecular diffusion

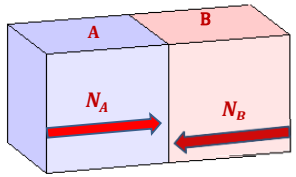
The term representing **bulk flow** $(N_A + N_B)\frac{C_A}{C}$

The term representing **Molecular diffusion** $-D_{AB}\frac{dC_A}{dz}$

If the concentration of ***A*** in a mixture is small (dilute solution), the contribution of bulk flow term become too small.

$$N_A = J_A = -D_{AB}\frac{dC_A}{dz} \qquad J_A = -CD_{AB}\frac{dy_A}{dz}$$

Proof of $D_{AB} = D_{BA}$ (Binary Diffusivity)



$$N_A = (N_A + N_B)y_A - CD_{AB}\frac{dy_A}{dz}$$

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

The total molar average concentration is C, If the gas mixture is ideal the mutual diffusivities of A and B are equal. So the flux of B in the mixture

$$N_B = (N_A + N_B)\frac{C_B}{C} - D_{BA}\frac{dC_B}{dz}$$

Net flux N

$$N = N_A + N_B$$

Combining the equation of Net flux N_A and N_B

$$N_A + N_B = (N_A + N_B)\left(\frac{C_A}{C} + \frac{C_B}{C}\right) - D_{AB}\frac{dC_A}{dz} - D_{BA}\frac{dC_B}{dz} = \text{Constant}$$

Again total concentration C is

$$C = C_A + C_B$$

and

$$\frac{dC_A}{dz} = -\frac{dC_B}{dz}$$

By putting all values in the above equation we will find

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

Steady state diffusion in fluids at rest / laminar Flow

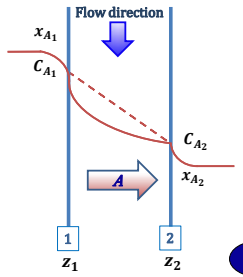
We know that $N_A = (N_A + N_B)\frac{C_A}{C} - D_{AB}\frac{dC_A}{dz}$

In case of diffusion only in the z- direction $\int_{C_{A1}}^{C_{A2}} \frac{-dC_A}{N_A C - C_A(N_A + N_B)} = \frac{1}{CD_{AB}}\int_{z_1}^{z_2} dz$

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, upon integration we get

$$\frac{1}{N_A + N_B} ln \frac{N_A C - C_{A_2}(N_A + N_B)}{N_A C - C_{A_1}(N_A + N_B)} = \frac{z}{CD_{AB}}$$

$$N_A = \frac{N_A}{N_A + N_B}\frac{D_{AB}C}{z} ln \frac{N_A/(N_A + N_B) - C_{A_2}/C}{N_A/(N_A + N_B) - C_{A_1}/C}$$



Molecular diffusion in gases

From ideal gas law,

For Liquid

For Gas

$$\frac{C_A}{C} = \frac{\bar{p}_A}{P} = y_A$$

Where:
$\bar{p}_A$ = Partial pressure of component ***A***
p_t = Total pressure
y_A = Mole fraction (concentration) of ***A***
R = Gas constant
T = Temperature

Further,

$$C = \frac{n}{V} = \frac{p_t}{RT}$$

$$N_A = \frac{N_A}{N_A + N_B} \frac{D_{AB}}{z} \frac{p_t}{RT} ln \frac{[N_A/(N_A + N_B)]p_t - \bar{p}_{A_2}}{[N_A/(N_A + N_B)]p_t - \bar{p}_{A_1}}$$

Finally,

$$N_A = \frac{N_A}{N_A + N_B} \frac{D_{AB}C}{z} \frac{p_t}{RT} ln \frac{N_A/(N_A + N_B) - y_{A_2}}{N_A/(N_A + N_B) - y_{A_1}}$$

Example

$$CH_4 \rightarrow C + 2H_2$$

CH_4 (A) is diffuses to the cracking surface and H_2 (B) diffuses back, the reaction stoichiometry fixes the relationship

$$N_B = -2N_A$$

Hence,

$$\frac{N_A}{N_A+N_B} = \frac{N_A}{N_A - 2N_A} = -1$$

In absence of chemical reaction, the ratio can be fixed by enthalpy considerations. In case of purely separation operations, there are two situations arises.

1. Diffusion of A through non-diffusing B $N_A = \text{Constan}, N_B = 0$ $\frac{N_A}{N_A+N_B} = 1$

2. Steady state Equimolar Counter Diffusion $N_A = -N_B \rightarrow (N_A+N_B) = 0$ $\frac{N_A}{N_A + N_B} = \infty$

References

ETH
Mass Transfer
Theories for Mass Transfer Coefficients
Lecture 9, 15.11.2017, Dr. K. Wegner

- Lecture notes/ppt of Dr. Yahya Banat (ybanat@qu.edu.qa)