Some definitions

Mass density, ρ_i [kg/m^3]: The amount of species i in a unit volume.

Molar concentration; C_i [$kmol/m^3$]: The amount of mole of species i in a unit volume.

If M_i [$kg/kmol$] is the molar weight of species i, relation between ρ_i and C_i as follows: $\rho_i = M_i C_i$

ρ_i represents the mass of species i per unit volume of the mixture, then the mixture density,

$$\rho = \sum \rho_i \quad \text{and} \quad C = \sum C_i$$

The amount of species i in the mixture may also be quantified as

$$m_i = \frac{\rho_i}{\rho}$$

and its mole fraction as

$$x_i = \frac{C_i}{C}$$

Then it follows that $\sum m_i = 1$ and $\sum x_i = 1$

Having $M_i = \frac{\rho_i}{C_i}$ also leads $M = \frac{\rho}{C}$ for mixture

$$M = \frac{\rho}{C} = \sum \frac{M_i C_i}{C} = \sum x_i M_i \text{ also.}$$

Exercise 9.1 of A.F. Mills (Basic Heat and Mass Transfer)

Derive equations: $m_i = \frac{x_i M_i}{\sum x_j M_j} = x_i \frac{M_i}{M}$ and $x_i = \frac{m_i / M_i}{\sum m_j / M_j} = m_i \frac{M}{M_i}$

$$m_i = \frac{\rho_i}{\rho} = \frac{\rho_i}{\sum \rho_i} \quad \text{where } C_i = \frac{\rho_i}{M_i} \rightarrow \rho_i = C_i M_i$$

$$\underline{m_i} = \frac{C_i M_i}{\sum C_i M_i} = \frac{C_i M_i}{\underbrace{\sum C_i}\sum M_i} = \frac{C_i}{C}\,\frac{M_i}{M} = \boxed{x_i \frac{M_i}{M}}$$

$$\boxed{x_i = \frac{C_i}{C} = \frac{\rho_i}{M_i}\,\frac{M}{\rho} = m_i \frac{M}{M_i}}$$

Fick law of diffusion

$$\boxed{J_i'' = -\rho D_{ij} \frac{dm_i}{dx}} \quad , \text{kg/m}^2\text{s : mass diffusion flux of species } i$$

$$J = J_i'' A \quad , D_{ij} : \text{Binary diffusion coefficient}$$

To express in molar base; having $C_i = \frac{\rho_i}{M_i}$ and $C = \frac{\rho}{M}$

$$J_i'' = -\rho D_{ij} \frac{dm_i}{dx} = -\rho D_{ij} \frac{d\frac{\rho_i}{\rho}}{dx} = -D_{ij} \frac{d\rho_i}{dx}$$

$$= -\rho D_{ij} \frac{d\left(\frac{C_i}{C}\frac{M_i}{M}\right)}{dx} = -\rho D_{ij} \frac{d\left(\frac{M_i}{M} x_i\right)}{dx}$$

$$= -\rho \frac{M_i}{M} D_{ij} \frac{dx_i}{dx}$$

$$\frac{J_i''}{M_i} = -C D_{ij} \frac{dx_i}{dx} \cdot \left[\frac{\text{kg}}{\text{s m}^2}\frac{\text{kmol}}{\text{kg}}\right]$$

$$\boxed{J_i''^{*} = -C D_{ij} \frac{dx_i}{dx}} \quad , \frac{\text{kmol}}{\text{m}^2\text{s}} \quad , \text{Fick law in molar base}$$

Permiability and Solubility:

Solubility S: Volume of solute gas dissolved in unit volume of solid [kmol/m³. bar]

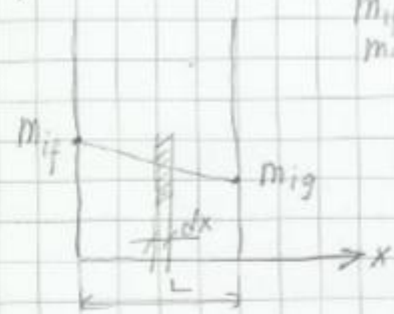
$$C_{i,\text{solid side}} = S_{i,\text{solid}} \cdot P_{i,\text{gas side}}$$

Permiability $\mathcal{P}_{i,s} = S_{is} \cdot D_{ij}$ (kmol/m.s. bar)

Then Fick's law interpretation in this concept;

Now let consider a plane wall;

m_{if} : Mass fraction in liquid side
m_{ig} : " " " gas side



$$J_i'' = -\rho D_{ij} \frac{dm_i}{dx} = \rho D_{ij} \frac{m_{if} - m_{ig}}{L} \quad kg/s.m^2$$

or in mol fraction base

$$\overset{*}{J}{}_i'' = C D_{ij} \frac{X_{i1} - X_{i2}}{L}$$

As solid is in between two gas mixture, the concentration of component of the gas in the solid is proportional with with the partical pressure of the adjacent gaz;

$C_{i,s} = S_{ij} \, P_{i,g}$

$\llcorner$ Solubility of i into j [kmol/m^3. bar]

Solubility is related with *diffusivity via permiability as*

$$\mathcal{P}_{ij} = S_{ij} \, D_{ij} \ [\text{kmol/m.s.bar}] \ : \text{Permiability}$$

Substituting these into the molar Fick law, one can obtain the equation as follows:

$$j_i'' = C \, D_{ij} \frac{X_{i1} - X_{i2}}{L} = \cancel{C} D_{ij} \frac{C_{i1} - C_{i2}}{\cancel{C} L} = D_{ij} \frac{C_{i1} - C_{i2}}{L}$$

Replacing C_{i1} & C_{i2} with $S_{ij} P_i$

$$\boxed{j_i'' = S_{ij} D_{ij} \frac{P_{i1} - P_{i2}}{L}}$$, where P_{i1} and P_{i2} are partial pressures of i at 1. & 2. regions -

or having $\mathcal{P}_{ij} = S_{ij} D_{ij}$

$$\boxed{j_i'' = \mathcal{P}_{ij} \frac{P_{i1} - P_{i2}}{L}}$$, kmol/m^2.s

Another form of Ficks law may be expressed for the ideal gases as

Example problem:

Hydrogen gas is maintained at 3 bar and 1 bar on opposite sides of a plastic membrane which is 0,3 mm thick. The temperature is 25°C, and the binary diffusion coefficient of hydrogen in the plastic is $8\times10^{-8}\ m^2/s$. The solubility of hydrogen in the membrane is 1.5×10^{-3} kmol/m³.bar, What is the mass diffusion flux of hydrogen through the membrane?

$D_{H_2-pls} = 8.7\times10^{-8}\ \frac{m^2}{s}$, $S_{H_2-pls} = 1.5\times10^{-3}$ kmol/m³.bar

$P_{H_2,1} = 3$ bar

$P_{H_2,2} = 1$ bar

$$j''_{H_2-plas} = \mathcal{P}_{H_2-pls}\frac{P_{H_2,1}-P_{H_2,2}}{L}$$

$$= 13.05\times10^{-11}\frac{(3-1)\,bar}{0.0003\,m}\cdot\frac{kmol}{m s.bar}$$

$L = 0.0003\ m$

$$j''_{H_2-pls} = 8.7\times10^{-7}\ \frac{kmol}{s.m^2}$$

$$\mathcal{P}_{H_2-pls} = S_{H_2-pls}\cdot D_{H_2-pls}$$

$$= 8.7\times10^{-8}\ \frac{m^2}{s}\cdot1.5\times10^{-3}\ \frac{kmol}{m^3 bar}$$

$$\mathcal{P} = 13.05\times10^{-11}\ \frac{kmol}{m.s.bar}$$

Since $J''_i = M j''_i$

$$J''_{H_2-pls} = M_{H_2}\cdot j''_{H_2-pls}$$

$$= 2\ \frac{kg}{kmol}\cdot 8.7\times10^{-7}\ \frac{kmol}{s.m^2} = 1.74\times10^{-6}\ kg/s.m^2$$

Some definitions on vapor air mixing

Relative humidity, $= \frac{m_v}{m_g}$,

Specific humidity, $\omega = \frac{m_v}{m_a}$

where

m_v: the vapor mass

m_g: the maximum vapor mass be able contained by the air at its existing temperature

m_a; air mass

Using the ideal gas relation and recognizing that volume and temperature are shared by both vapor and air, we will have;

$m_v = \frac{P_v V}{R_v T}$ and $m_a = \frac{P_a V}{R_a T}$

Evaluating for specific humidity for R_a = 287 J/kgK and R_v = 461 J/kgK

$$\omega = \frac{P_v \cancel{V}}{R_v \cancel{T}} \frac{R_a \cancel{T}}{P_a \cancel{V}} = \frac{R_a}{R_v} \frac{P_v}{P_a} = 0.622 \frac{P_v}{P_a} = \frac{0.622 x P_v}{P - P_v}$$

Since RH is also defined as $RH = \frac{P_v}{P_{sat@T}}$, then

$$\omega = \frac{0.622 x RH x P_{sat@T}}{P - P_{sat@T}}$$

Obtaining RH,

$$RH = \frac{\omega x P}{(0.622 + \omega) P_{sat@T}}$$