Ch 17. Diffusion and Mechanisms of Mass Transport

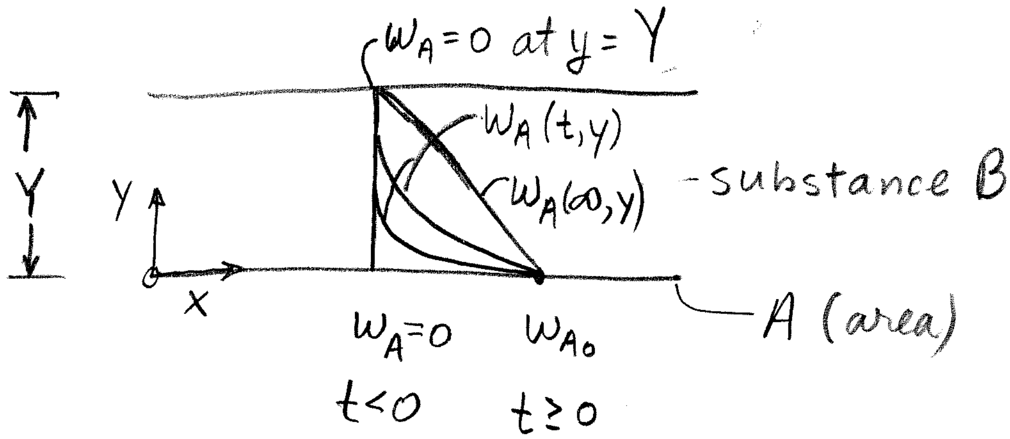
17.1 Fick's Law of Binary Diffusion (Molecular Mass Transport).

Binary diffusion is the net transport of one species (A) through another species (B) by a concentration gradient.

analogous terms

- mass diffusion, concentration diffusion, ordinary diffusion.

Consider a slab of material (B)



$$w_A = \frac{\text{mass of } A}{\text{mass } A + \text{mass } B}$$, in a unit volume

W_{Ay} = mass flow of A in +y direction

Fick's 1st Law:

$$\frac{W_{Ay}}{A} = \rho \mathcal{D}_{AB}\left(\frac{w_{A0}-0}{Y}\right)$$

ρ = density of the species A, B system (g/cm^3)
$\mathcal{D}_{AB}$ = diffusivity of A through B (cm^2/s)

For a differential elemental volume within the slab,

$$\boxed{j_{Ay} = -\rho \mathcal{D}_{AB} \frac{\partial w_A}{\partial y}}$$

j_{Ay} = molecular mass flux of A in +y direction
(j_{Ay} is relative to the mixture velocity, v_y)

$$v_y = w_A v_{Ay} + w_B v_{By}$$

where v_A and v_B are arithmetic averages of the molecular velocities within a volume element.

$$j_{Ay} = \rho w_A (v_{AY} - v_y)$$

if A were diffusing through a solid (B), $v_{By}=0$

$$v_y = \omega_A v_{Ay} + \omega_B(0) = \omega_A v_{Ay}.$$

and $$j_{Ay} = \rho\omega_A(v_{Ay} - \omega_A v_{Ay}) = \rho\omega_A v_{Ay}(1-\omega_A)$$

$$j_{By} = \rho\omega_B(v_{By} - v_y) = \rho\omega_B(0 - \omega_A v_{Ay})$$

$$= \rho(1-\omega_A)(-\omega_A v_{Ay}) = -\rho\omega_A v_{Ay}(1-\omega_A)$$

thus $\boxed{j_{Ay} = -j_{By}}$ when the fluxes are defined relative to v_y!

This a general result - not just for diffusion in a solid.

If gradients of A occur in all 3 coordinate directions,

$$\boxed{j_A = -\rho \mathcal{D}_{AB} \nabla \omega_A}$$ a vector equation

If the material through which A is diffusing allows for preferrential diffusion in certain directions

$$\boxed{j_A = -[\rho \Delta_{AB} \cdot \nabla \omega_A]}$$

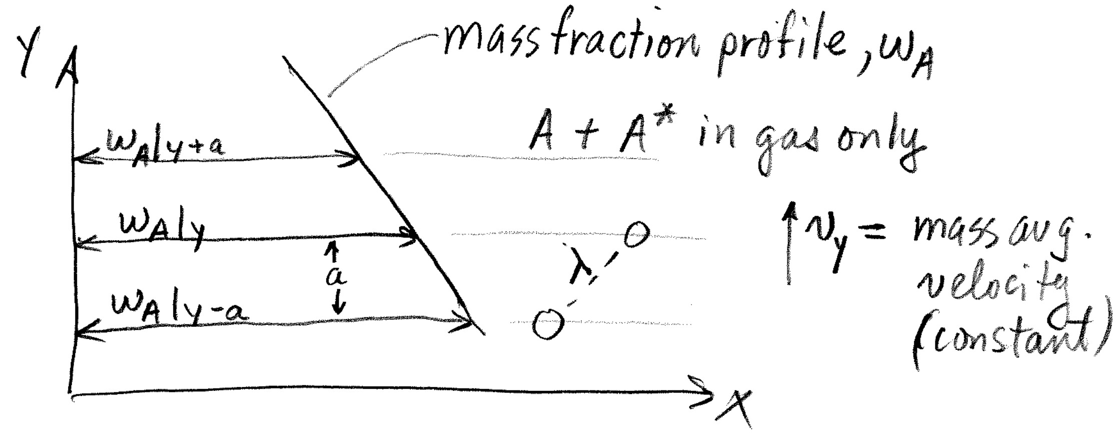
in which Δ_{AB} is a symmetric diffusivity tensor (for some polymeric liquids or structured solids).

Tables 17.1, 2, 3, and 4 contain $\mathcal{D}_{AB}$ values

$$\mathcal{D}_{AB} = f(T, p, w_A \text{ or } x_A)$$

↳ mole fraction A

17.3 Kinetic Theory of Diffusion in Gases: Low Density



A^* is identical to A except it has a label: e.g. radioactive.

- kinetic theory relations

$$\bar{u} = \sqrt{\frac{8KT}{\pi m}}, \quad Z_A = \frac{1}{2} n_A \bar{u}, \quad \lambda = \frac{1}{\sqrt{2}\,\pi d^2 n}$$

(n_A = number concentration of A)

$$a = \frac{2}{3}\lambda$$

Mass of A crossing a plane at $y=y$ in $+y$-direction

$$\div \tilde{N} \times M_A \quad \underbrace{(\overbrace{\rho w_A}^{n_A} v_y)}_{\text{convective mass flow/area}} + \underbrace{\left[\left(\tfrac{1}{4}\overbrace{\rho w_A}^{n_A}\bar{u}\right)\Big|_{y-a} - \left(\tfrac{1}{4}\overbrace{\rho w_A}^{n_A}\bar{u}\right)\Big|_{y+a}\right]}_{\text{net transport of mass of A by molecular motions / area}}$$

Assuming dw_A/dy is linear over a distance a,

$$w_A|_{y-a} = w_A|_y - \frac{2}{3}\lambda\frac{dw_A}{dy}$$

$$w_A|_{y+a} = w_A|_y + \frac{2}{3}\lambda\frac{dw_A}{dy}$$

Subst. in above,

$$(\rho w_A v_y) + \left[\frac{1}{4}\rho\bar{u}\left(w_A|_y - \frac{2}{3}\lambda\frac{dw_A}{dy}\right) - \frac{1}{4}\rho\bar{u}\left(w_A|_y + \frac{2}{3}\lambda\frac{dw_A}{dy}\right)\right]$$

$$\boxed{(\rho w_A v_y) - \frac{1}{3}\rho\bar{u}\lambda\frac{dw_A}{dy} = n_{Ay}} \boxed{\equiv \rho w_A v_y - \rho \mathcal{D}_{AA^*}\frac{dw_A}{dy}}$$

$$\therefore \boxed{\mathcal{D}_{AA^*} = \frac{1}{3}\lambda\bar{u}}$$

$$\mathcal{D}_{AA^*} = \frac{1}{3} \cdot \frac{1}{\sqrt{2}\,\pi d_A^2 n} \cdot \sqrt{\frac{8KT}{\pi m_A}}$$

$$\boxed{= \frac{2}{3\pi} \cdot \frac{\sqrt{\pi m_A K T}}{\pi d_A^2} \; \frac{1}{\rho}}$$

note $\underline{n m_A = \rho}$ m_A = mass of atom$_A$.

Result for $A \neq B$.

$$\boxed{\mathcal{D}_{AB} = \frac{2}{3} \sqrt{\frac{KT}{\pi}} \sqrt{\frac{1}{2}\left(\frac{1}{m_A} + \frac{1}{m_B}\right)} \; \frac{1}{\pi\left(\frac{1}{2}(d_A + d_B)\right)^2} \; \frac{1}{n}}$$

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