17.7 Convection Transport of Mass/Moles.

Convective mass flux vector $\rightarrow \rho_A v$

ρ_A = mass concentration (g/cm^3)

v = mass average velocity

$$= \frac{\sum_{\alpha=1}^{N} \rho_\alpha v_\alpha}{\sum_{\alpha=1}^{N} \rho_\alpha} = \frac{\sum_{\alpha=1}^{N} \rho_\alpha v_\alpha}{\rho} = \sum_{\alpha=1}^{N} w_A v_\alpha$$

v_α = species "α" velocity relative to stationary coord.

convective molar flux vector $\rightarrow c_A v^*$

c_A = molar concentration ($moles/cm^3$)

v^* = molar average velocity $= \sum_{\alpha=1}^{N} x_\alpha v_\alpha$

$$x_\alpha = \frac{c_\alpha}{c} = \frac{c_\alpha}{\sum_{\alpha=1}^{N} c_\alpha}$$

Molecular Mass or Molar Fluxes.

$$\text{Mass:} \quad j_A = \rho_A(v_A - v) = -\rho \mathcal{D}_{AB} \nabla w_A$$

$$\text{Molar:} \quad J_A^* = c_A(v_A - v^*) = -c\mathcal{D}_{AB} \nabla x_A$$

Combined Mass/Mole Fluxes

$$\text{Mass:} \quad n_A = j_A + \rho_A v$$

$$\text{Molar:} \quad N_A = J_A^* + c_A v^*$$

Other Relationships:

$$\text{sum of mass fluxes:} = \sum_{\alpha=1}^{N} n_\alpha = \sum_{\alpha=1}^{N} \rho_\alpha v_\alpha = \sum_{\alpha=1}^{N} \rho w_\alpha v_\alpha$$

$$= \rho \sum_{\alpha=1}^{N} w_\alpha v_\alpha = \boxed{\rho v}$$

$$\text{sum of molar fluxes} = \sum_{\alpha=1}^{N} N_\alpha = \sum_{\alpha=1}^{N} c_\alpha v_\alpha = \sum_{\alpha=1}^{N} c x_\alpha v_\alpha$$

$$= c \sum_{\alpha=1}^{N} x_\alpha v_\alpha = \boxed{c v^*}$$

revisit sum of mass fluxes

$$\sum_{\alpha=1}^{N} n_\alpha = \rho v \qquad \text{from above.}$$

$$\sum_{\alpha=1}^{N} (j_\alpha + \rho_\alpha v) = \rho v$$

$$\sum_{\alpha=1}^{N} j_\alpha + \sum_{\alpha=1}^{N} \rho_\alpha v = \rho v$$

$$\sum_{\alpha=1}^{N} j_\alpha + \cancel{\rho v} = \cancel{\rho v} \Rightarrow \boxed{\sum_{\alpha=1}^{N} j_\alpha = 0}$$

Molar Fluxes $\boxed{\sum_{\alpha=1}^{N} J_\alpha^* = 0}$

revisit combined mass/molar fluxes.

mass:
$$n_A = j_A + \rho_A v$$
$$= j_A + \omega_A \rho v$$
$$\boxed{= j_A + \omega_A \sum_{\alpha=1}^{N} n_\alpha}$$

molar:
$$\boxed{N_A = J_A^* + x_A \sum_{\alpha=1}^{N} N_\alpha}$$

Binary Systems , A + B.

Table 17.8-2 summarizes relationships.

Ch. 18 Concentration Distributions in Solids & Laminar Flow

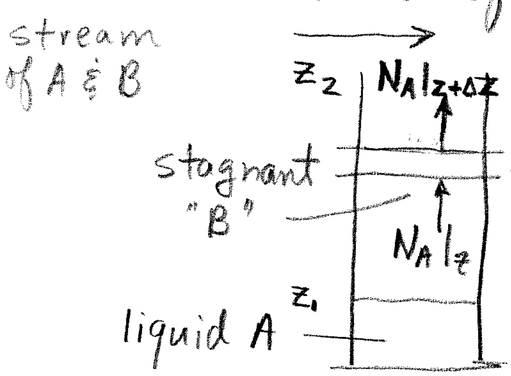
Binary Systems:

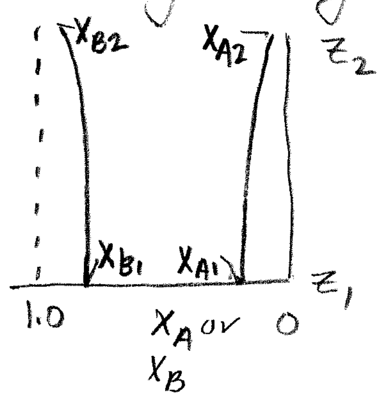
$$N_A = -c\mathcal{D}_{AB}\nabla x_A + x_A(N_A + N_B)$$

Conservation of Mass.

rate of mass A in − rate of mass A out + rate of production of A = 0

18.2 Diffusion of "A" Through Stagnant "B".





$$\boxed{\begin{aligned} N_A &= f(z) \text{ only} \\ &= N_{Az} \end{aligned}}$$

at z_1, liquid evaporates to establish a partial pressure of "A", P_A^{vap} $\therefore$ $x_{A1} = \dfrac{P_A^{vap}}{P}$

assuming Ideal Gas.

Consider the Combined Flux of A, when $N_B = 0$ (stagnant "B")

$$N_{Az} = -c\mathcal{D}_{AB}\frac{\partial x_A}{\partial z} + x_A\left(N_{Az} + \cancel{N_{Bz}}^{\,0}\right)$$

"a convective transport induced by diffusion!"

$$\therefore \boxed{N_{Az} = -\frac{c\mathcal{D}_{AB}}{(1-x_A)}\frac{\partial x_A}{\partial z}}$$

Combined Flux of B;

$$\cancel{N_{Bz}}^{\,0} = -c\mathcal{D}_{AB}\frac{\partial x_B}{\partial z} + x_B\left(N_{Az} + \cancel{N_{Bz}}^{\,0}\right)$$

$$\therefore \boxed{\frac{\partial x_B}{\partial z} = \frac{x_B N_{Az}}{c\mathcal{D}_{AB}}}$$

thus a gradient in "B" is induced by N_{Az}.

$$= \frac{x_B\left(-\frac{\cancel{c\mathcal{D}_{AB}}}{1-x_A}\frac{dx_A}{dz}\right)}{\cancel{c\mathcal{D}_{AB}}} = -\frac{x_B}{1-x_A}\frac{dx_A}{dz}$$

$$= -\frac{1-x_A}{1-x_A}\frac{dx_A}{dz} = \boxed{-\frac{dx_A}{dz}}$$

Shell Mole Balance

$$S\,N_{Az}|_z - S\,N_{Az}|_{z+\Delta z} = 0$$

S = cross-sectional area of tube

$\div$ by $S \cdot \Delta z$ let $\Delta z \to 0$.

$$-\frac{dN_{Az}}{dz} = 0$$

since $N_{Az} = -\frac{c\mathcal{D}_{AB}}{1-x_A}\frac{dx_A}{dz}$

$$\frac{d}{dz}\left(\frac{c\mathcal{D}_{AB}}{1-x_A}\frac{dx_A}{dz}\right) = 0$$

$$\frac{d}{dz}\left(\frac{1}{1-x_A}\frac{dx_A}{dz}\right) = 0$$

for T & P constant and Ideal Gas, c is constant. Also, $\mathcal{D}_{AB}$ ~ constant though x_A changes.

Integrating Once, $\frac{1}{1-x_A}\frac{dx_A}{dz} = C_1$

Again $-\ln(1-x_A) = C_1 z + C_2$ (18.2-7)

Replace $C_1 = -\ln K_1$ $\quad C_2 = -\ln K_2$

18.2-7 becomes $1-x_A = K_1^z K_2$

BC1	$z = z_1$	$x_A = x_{A1}$
BC2	$z = z_2$	$x_A = x_{A2}$

$$1-X_{A1} = K_1^{z_1} K_2 \qquad \underline{BC1}$$

$$1-X_{A2} = K_1^{z_2} K_2 \qquad BC2$$

Ratio of BC1 ÷ by BC2.

$$\left(\frac{1-X_{A1}}{1-X_{A2}}\right) = K_1^{(z_1-z_2)} \Rightarrow \boxed{K_1 = \left(\frac{1-X_{A1}}{1-X_{A2}}\right)^{\frac{1}{(z_1-z_2)}}}$$

From BC1 eqn.

$$1-X_{A1} = K_1^{z_1} K_2 \Rightarrow K_2 = \frac{1-X_{A1}}{K_1^{z_1}}$$

$$\boxed{K_2 = \frac{1-X_{A1}}{\left(\frac{1-X_{A1}}{1-X_{A2}}\right)^{z_1/(z_1-z_2)}}}$$

$$1-X_A = K_1^{z} K_2 = \left(\frac{1-X_{A1}}{1-X_{A2}}\right)^{z/(z_1-z_2)} \frac{1-X_{A1}}{\left(\frac{1-X_{A1}}{1-X_{A2}}\right)^{z_1/(z_1-z_2)}}$$

$$\frac{1-X_A}{1-X_{A1}} = \left(\frac{1-X_{A1}}{1-X_{A2}}\right)^{\frac{z-z_1}{z_1-z_2}}$$

$$\boxed{= \left(\frac{1-X_{A2}}{1-X_{A1}}\right)^{(z-z_1)/(z_2-z_1)}}$$

or

$$\frac{X_B}{X_{B1}} = \left(\frac{X_{B2}}{X_{B1}}\right)^{\frac{z-z_1}{z_2-z_1}}$$

Rate of Transfer of Moles at Interface.

$$N_{Az}\Big|_{z=z_1} = -\frac{c\mathcal{D}_{AB}}{1-x_{A1}}\frac{dx_A}{dz}\Big|_{z=z_1} = +\frac{c\mathcal{D}_{AB}}{x_{B1}}\frac{dx_B}{dz}\Big|_{z=z_1}$$

but $\displaystyle \frac{dx_B}{dz}\Big|_{z_1} = x_{B1}\frac{d}{dz}\left(\frac{x_{B2}}{x_{B1}}\right)^{(z-z_1)/(z_2-z_1)}$

$$= x_{B1}\left(\frac{x_{B2}}{x_{B1}}\right)^{(z_1-z_1)/(z_2-z_1)} \ln\left(\frac{x_{B2}}{x_{B1}}\right)\cdot\frac{1}{(z_2-z_1)}$$

$$= x_{B1}\ln\left(\frac{x_{B2}}{x_{B1}}\right)\cdot\frac{1}{(z_2-z_1)}$$

$$N_{Az}\Big|_{z=z_1} = \frac{c\mathcal{D}_{AB}}{x_{B1}}\cdot x_{B1}\ln\left(\frac{x_{B2}}{x_{B1}}\right)\cdot\frac{1}{(z_2-z_1)}$$

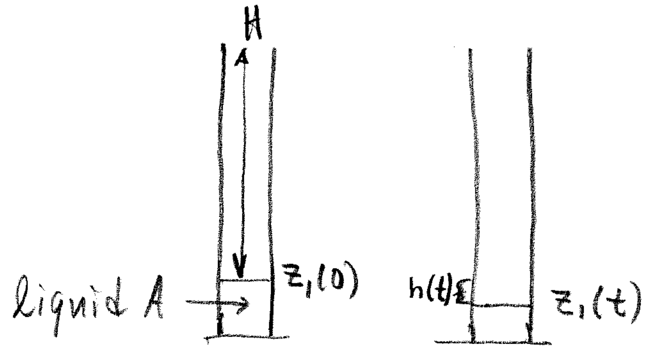
$$= \frac{c\mathcal{D}_{AB}}{z_2-z_1}\ln\left(\frac{x_{B2}}{x_{B1}}\right).$$

but $\displaystyle (x_B)_{ln} = \frac{x_{B2}-x_{B1}}{\ln(x_{B2}/x_{B1})}$

$$\therefore \ln\left(\frac{x_{B2}}{x_{B1}}\right) = \frac{x_{B2}-x_{B1}}{(x_B)_{ln}} = \frac{1-x_{A1}-1+x_{A2}}{(x_B)_{ln}} = \frac{x_{A2}-x_{A1}}{(x_B)_{ln}}$$

$$\boxed{N_{Az}\Big|_{z=z_1} = \frac{c\mathcal{D}_{AB}}{(z_2-z_1)}\frac{(x_{A2}-x_{A1})}{(x_B)_{ln}}}$$

Example 18.2-1 Diffusion With a Moving Interface.



assume that the diffusion occurs at quasi-steady-state.

$$N_{Az}\big|_{z_1} = \frac{c\mathcal{D}_{AB}}{(z_2 - z_1(t))} \cdot \frac{x_{A1} - x_{A2}}{(x_B)_{ln}}$$

$$-S\frac{\rho^{(A)}}{M_A}\frac{dz_1}{dt} = N_{Az}\big|_{z_1} \cdot S = \frac{c\mathcal{D}_{AB}}{(z_2 - z_1(t))} \cdot \frac{x_{A1} - x_{A2}}{(x_B)_{ln}}$$

$$-(z_2 - z_1(t))\, dz_1 = \frac{c\mathcal{D}_{AB}}{(\rho^{(A)}/M_A)} \cdot \frac{(x_{A1} - x_{A2})}{(x_B)_{ln}} \cdot dt$$

but $H = z_2 - z_1(0)$ or $z_2 = H + z_1(0)$

$h(t) = z_1(0) - z_1(t)$ or $z_1(t) = z_1(0) - h(t)$

$$-(H + z_1(0) - z_1(0) + h(t))(-dh) = \frac{c\mathcal{D}_{AB}}{(\rho^{(A)}/M_A)} \cdot \frac{(x_{A1} - x_{A2})}{(x_B)_{ln}}\, dt$$

$$\int_0^h (H + h)\, dh = \frac{c\mathcal{D}_{AB}(x_{A1} - x_{A2})}{(\rho^{(A)}/M_A)(x_B)_{ln}} \int_0^t dt$$

$$Hh + \frac{1}{2}h^2 = \frac{c\mathcal{D}_{AB}(x_{A1} - x_{A2})}{(\rho^{(A)}/M_A)(x_B)_{ln}}\, t = \frac{1}{2}Ct$$

where $C = \dfrac{2c\,\mathcal{D}_{AB}(x_{A1}-x_{A2})}{(\rho^{(A)}/M_A)(x_B)_{ln}}$

quadratic eqn is

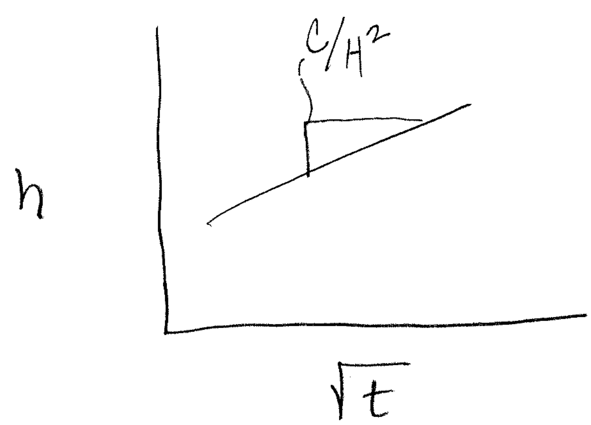
$$h^2 + 2Hh - Ct = 0$$

$$h = \frac{-2H \pm \sqrt{4H^2+4Ct}}{2(1)} = \frac{\pm\cancel{2}\sqrt{H^2+Ct} - \cancel{2}H}{\cancel{2}}$$

only + roots

$$\boxed{h = H\left(\sqrt{1+Ct/H^2} - 1\right)}$$

Measuring h vs t, $\mathcal{D}_{AB}$ can be obtained.



$\underline{\mathcal{D}_{AB} = f(C)}$.

Mon
4/3/06