Multicomponent Diffusion: Gases at Low Density

$$\nabla x_\alpha = -\sum_{\beta=1}^{N} \frac{x_\alpha x_\beta}{\mathcal{D}_{\alpha\beta}}(v_\alpha - v_\beta) = -\sum_{\beta=1}^{N} \frac{1}{c\mathcal{D}_{\alpha\beta}}(x_\beta N_\alpha - x_\alpha N_\beta)$$

"Maxwell-Stephan Equations" (17.9-1)

<u>Binary Diffusion</u>, (A+B)

$$\nabla x_A = -\frac{x_A x_B}{\mathcal{D}_{AB}}(v_A - v_B) = -\frac{1}{c\mathcal{D}_{AB}}(x_B N_A - x_A N_B)$$

$$-c\mathcal{D}_{AB}\nabla x_A = x_B N_A - x_A N_B = (1-x_A)N_A - x_A N_B$$

$$= N_A - x_A N_A - x_A N_B$$

$$= N_A - x_A(N_A + N_B)$$

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

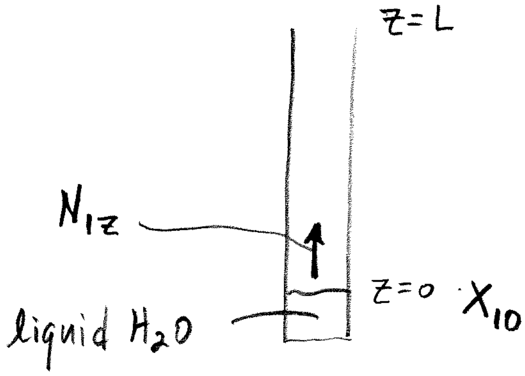
Ternary System, (A+B+C)

$$\nabla x_A = -\frac{1}{c\mathcal{D}_{AB}}(x_B N_A - x_A N_B) - \frac{1}{c\mathcal{D}_{AC}}(x_C N_A - x_A N_C)$$

$$\nabla x_C = -\frac{1}{c\mathcal{D}_{AC}}(x_A N_C - x_C N_A) - \frac{1}{c\mathcal{D}_{BC}}(x_B N_C - x_C N_B)$$

Ternary Diffusion in the Evaporation Tube. (18.8)

$x_{1L} = .1, \; x_{2L} = .75, \; x_{3L} = .15$



Species 1 = H_2O vapor
" 2 = N_2
" 3 = O_2

$p = 1$ atm.

$T = 352\,K$

$P_{H_2O}(352K) = 341$ mm Hg

$x_{10} = 341/760 = .449$

Conservation of Mass.

$$\frac{dN_{1z}}{dz} = 0, \quad \frac{dN_{2z}}{dz} = 0, \quad \frac{dN_{3z}}{dz} = 0$$

Stagnant 2,3 , $N_{2z} = N_{3z} = 0$

Sum of Mole Fractions: $x_1 + x_2 + x_3 = 1$

from which we obtain $x_1 = 1 - x_2 - x_3$

Molar Flux Expressions: "Maxwell-Stephan" Eqns.

$$N_2: \quad \frac{dx_2}{dz} = -\frac{1}{c\mathcal{D}_{21}}\left(x_1 \overset{0}{N_{2z}} - x_2 N_{1z}\right) - \frac{1}{c\mathcal{D}_{23}}\left(x_3 \overset{0}{N_{2z}} - x_2 \overset{0}{N_{3z}}\right)$$

$$\frac{dx_2}{dz} = \frac{N_{1z}}{c\mathcal{D}_{21}} x_2 \longrightarrow \int_{x_2}^{x_{2L}} \frac{dx_2}{x_2} = \frac{N_{1z}}{c\mathcal{D}_{12}} \int_z^L dz$$

$$\boxed{\frac{x_2}{x_{2L}} = \exp\left(-\frac{N_{1z}(L-z)}{c\mathcal{D}_{12}}\right).}$$

$$O_2: \quad \frac{dx_3}{dz} = -\frac{1}{c\mathcal{D}_{31}}\left(x_1 \cancelto{0}{N_{3z}} - x_3 N_{1z}\right) - \frac{1}{c\mathcal{D}_{32}}\left(x_2 \cancelto{0}{N_{3z}} - x_3 \cancelto{0}{N_{2z}}\right)$$

$$\frac{dx_3}{dz} = \frac{N_{1z}}{c\mathcal{D}_{13}} x_3 \longrightarrow \int_{x_3}^{x_{3L}} \frac{dx_3}{x_3} = \frac{N_{1z}}{c\mathcal{D}_{13}} \int_z^L dz$$

$$\boxed{\frac{x_3}{x_{3L}} = \exp\left(-\frac{N_{1z}(L-z)}{c\mathcal{D}_{13}}\right)}$$

$$H_2O: \quad x_1 = 1 - x_2 - x_3$$

$$\boxed{x_1 = 1 - x_{2L}\exp\left(-\frac{N_{1z}(L-z)}{c\mathcal{D}_{12}}\right) - x_{3L}\exp\left(-\frac{N_{1z}(L-z)}{c\mathcal{D}_{13}}\right)}$$

But what is N_{1z}?

at $z=0$ $\quad x_1 = x_{10} = .449.$

$$\boxed{x_{10} = 1 - x_{2L}\exp\left(-\frac{N_{1z}L}{c\mathcal{D}_{12}}\right) - x_{3L}\exp\left(-\frac{N_{1z}L}{c\mathcal{D}_{13}}\right)}$$

N_{1z} can be found by, for example, trial + error!

$$\mathcal{D}_{12} = .364\ \frac{cm^2}{s} \qquad \mathcal{D}_{13} = .357\ \frac{cm^2}{s}$$

If we assume $\mathcal{D}_{12} = \mathcal{D}_{13} = .36.$

$$x_{10} = 1 - .90\exp\left(-\frac{N_{1z}L}{c\mathcal{D}_{12}}\right)$$

$$.90\exp\left(-\frac{N_{1z}L}{c\mathcal{D}_{12}}\right) = 1 - x_{10}$$

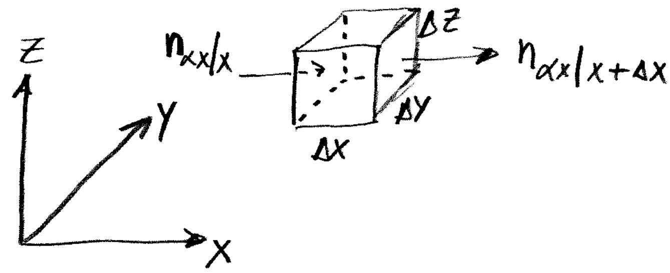
$$-\frac{N_{1z}L}{c\mathcal{D}_{12}} = \ln\left(\frac{1-x_{10}}{.90}\right)$$

$$\boxed{N_{1z} = \frac{c\mathcal{D}_{12}}{L}\ln\left(\frac{.9}{1-x_{10}}\right)}$$

$$= \frac{(3.46\times10^{-5}\ g\text{-moles}/cm^3)(.36\ \frac{cm^2}{s})}{(11.2\ cm)}\ln\left(\frac{.9}{1-.449}\right)$$

$$\boxed{= 5.46\times10^{-7}\ \frac{g\cdot moles}{cm^2\cdot s}}$$

Ch 19. Eqn.s of Change For Multicomponent Systems



accumulation of mass (α)	$(\partial \rho_\alpha/\partial t)\,\Delta x \Delta y \Delta z$
x-component of n_α vector	$(n_{\alpha x}\|_x - n_{\alpha x}\|_{x+\Delta x})\,\Delta y\,\Delta z$
y- " " " "	$(n_{\alpha y}\|_y - n_{\alpha y}\|_{y+\Delta y})\,\Delta x\,\Delta z$
z- " " " "	$(n_{\alpha z}\|_z - n_{\alpha z}\|_{z+\Delta z})\,\Delta x\,\Delta y$
rate of production of α	$r_\alpha\,\Delta x\,\Delta y\,\Delta z$

$$\frac{\partial \rho_\alpha}{\partial t} = -\left(\frac{\partial n_{\alpha x}}{\partial x} + \frac{\partial n_{\alpha y}}{\partial y} + \frac{\partial n_{\alpha z}}{\partial z}\right) + r_\alpha \qquad (19.1\text{-}5)$$

$$\frac{\partial \rho_\alpha}{\partial t} = -(\nabla \cdot n_\alpha) + r_\alpha \qquad (19.1\text{-}6)$$

where $n_\alpha = \rho_\alpha v_\alpha$ $\qquad \alpha = 1, 2, 3 \ldots N$

Summing $\sum_{\alpha=1}^{N}$ (19.1-6) $\rightarrow$ $\boxed{\dfrac{\partial \rho}{\partial t} = -(\nabla \cdot \rho v)}$

where $\sum_{\alpha=1}^{N} n_\alpha = \rho v$ (Table 17.8-1) $\quad \sum_{\alpha=1}^{N} r_\alpha = 0$

for a fluid of constant ρ $\Rightarrow$ $\boxed{(\nabla \cdot v) = 0}$

Substituting $n_\alpha = j_\alpha + \rho_\alpha v$

$$\boxed{\frac{\partial \rho_\alpha}{\partial t} = -(\nabla \cdot \rho_\alpha v) - (\nabla \cdot j_\alpha) + r_\alpha} \qquad \alpha = 1, 2, 3, \ldots N$$

→ Table B.10

$$j_\alpha \equiv -\rho \mathcal{D}_{AB} \nabla w_\alpha$$

Molar Form - Eqn. of Continuity For Species α.

$$\boxed{\frac{\partial c_\alpha}{\partial t} = -(\nabla \cdot c_\alpha v^*) - (\nabla \cdot J^*_\alpha) + R_\alpha} \qquad (19.1\text{-}11) \quad \alpha = 1, 2, 3, \ldots N$$

Summing over all α.

$$\frac{\partial c}{\partial t} = -(\nabla \cdot c v^*) + \sum_{\alpha=1}^{N} R_\alpha \qquad (19.1-12)$$

Expanding 1st term on r.h.s. of 19.1-11

$$\frac{\partial c_\alpha}{\partial t} = -c_\alpha(\nabla \cdot v^*) - (v^* \cdot \nabla c_\alpha) - (\nabla \cdot J^*_\alpha) + R_\alpha$$

or

$$\frac{\partial c_\alpha}{\partial t} + c_\alpha(\nabla\cdot V^*) + (V^*\cdot\nabla c_\alpha) = -(\nabla\cdot J_\alpha^*) + R_\alpha$$

let $c_\alpha = c\,x_\alpha$

$$c\frac{\partial x_\alpha}{\partial t} + x_\alpha\frac{\partial c}{\partial t} + x_\alpha c(\nabla\cdot V^*) + c(V^*\cdot\nabla x_\alpha) + x_\alpha(V^*\cdot\nabla c) = -(\nabla\cdot J_\alpha^*) + R_\alpha$$

Rearranging,

$$c\left(\frac{\partial x_\alpha}{\partial t} + (V^*\cdot\nabla x_\alpha)\right) + x_\alpha\left(\frac{\partial c}{\partial t} + \underbrace{c(\nabla\cdot V^*) + (V^*\cdot\nabla c)}_{(\nabla\cdot cV^*)}\right) = -(\nabla\cdot J_\alpha^*) + R_\alpha$$

$$\sum_{\alpha=1}^{N} R_\alpha$$

$$\boxed{c\left(\frac{\partial x_\alpha}{\partial t} + (V^*\cdot\nabla x_\alpha)\right) = -(\nabla\cdot J_\alpha^*) + R_\alpha - x_\alpha\sum_{\alpha=1}^{N} R_\alpha} \quad (19.1\text{-}15)$$

Similarly for Mass Concentrations,

$$\boxed{\rho\left(\frac{\partial w_\alpha}{\partial t} + (v\cdot\nabla w_\alpha)\right) = -(\nabla\cdot j_\alpha) + r_\alpha} \quad (19.1\text{-}14)$$

Now For Binary Systems (A + B only!)

For Constant $\rho \mathcal{D}_{AB}$ (dilute fluid systems , $w_A \sim 0$)

$$\left.\rho\left(\frac{\partial w_A}{\partial t} + (v \cdot \nabla w_A)\right) = \rho \mathcal{D}_{AB} \nabla^2 w_A + r_A \right\}$$ Table B.11

For Constant $c\mathcal{D}_{AB}$ ($x_A \sim 0$)

$$c\left(\frac{\partial x_A}{\partial t} + (v^* \cdot \nabla x_A)\right) = c\mathcal{D}_{AB} \nabla^2 x_A + R_A - x_A R_A - x_{\cancel{X}} R_B$$

$$= c\mathcal{D}_{AB} \nabla^2 x_A + x_B R_A - x_A R_B$$

For Zero Velocity / No Reaction: $v, v^* = 0$ $r_A, R_A = 0$.
c, ρ constant.

$$\boxed{\frac{\partial c_A}{\partial t} = \mathcal{D}_{AB} \nabla^2 c_A}$$ Fick's Second Law of Diffusion

Mon. 04/10/06