Lecture 16–17: Species Mass Transport, Shell Balances

I. Mass Transport Shell Balances

II. Diffusion of gas in a solid (Ex.)

- Boundary Conditions

III. Ex. Diffusion through a stagnant gas film ← We are here.

A. "Intuitive" choices for $\underline{n}_A, \underline{n}_B, \underline{v}$

B. Example w/ full math

IV. Chemical Reactions

III. Example: Diffusion through a stagnant film

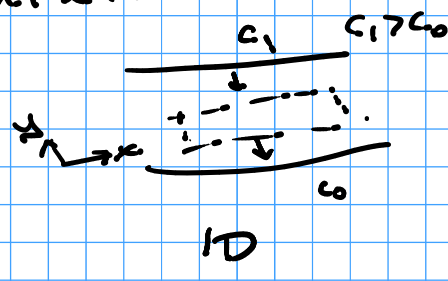
$$* \quad \underline{n}_A = \rho_A \underline{v} + \underline{j}_A$$

$$\underline{n}_B = \rho_B \underline{v} + \underline{j}_B$$

$$\rho \underline{v} = \underline{n}_A + \underline{n}_B \leftarrow$$

A. "Intuitive" choices for $\underline{n}_A, \underline{n}_B, \underline{v}$.

* consider <u>any</u> s.s. binary mixture w/o a generation term



$$\frac{d}{dy} n_{A,y} = 0 \leftarrow \text{when}$$

$$\Downarrow$$

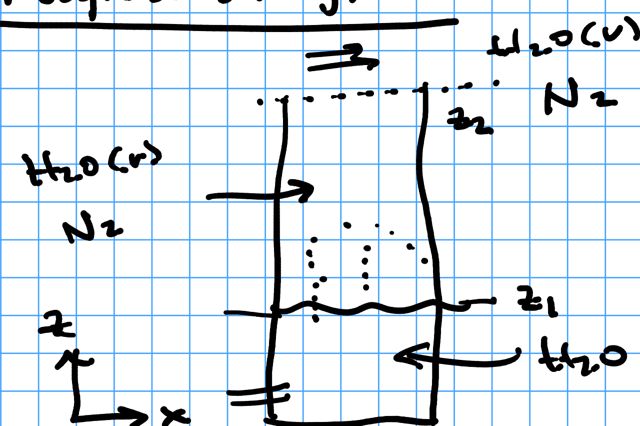
$$n_{A,y} = \text{const}$$

$$\frac{d}{dy} n_{B,y} = 0 \Rightarrow n_{B,y} = \text{const}$$

* In this "intuitive" way to solve M.T. Balances we get the following cases:

- $\underline{v} = 0$ (e.g. medium is a solid)
- $\underline{n}_A = 0$ or $\underline{n}_B = 0$ (e.g. a stagnant species)
- $\underline{n}_A = \underline{n}_A|_{boundary}$ or $\underline{n}_B = \underline{n}_B|_{boundary}$ (e.g. chem rxn)

B. Ex. Diffusion through a stagnant gas film



(1) what is the concentration of N_2, $H_2O(v)$?

$A = H_2O(v)$

$B = N_2$

top: x_{A2} x_{B2}

bottom: x_{A1} x_{B1}

(2-3) write bal. equation

$$\frac{dN_{Az}}{dz} = 0 \qquad \frac{dN_{Bz}}{dz} = 0$$

$$\underline{N}_A = c_A \underline{v}^* + \underline{J}_A^*$$

$$\underline{N}_B = c_B \underline{v}^* + \underline{J}_B^*$$

$$c\underline{v}^* = \underline{N}_A + \underline{N}_B$$

- lets look at B first:

$$N_{B,z} = c_1 \qquad N_{B,z}\big|_{z_1} = 0$$

$$= 0$$

- Back to A:

$$\frac{dN_{A,z}}{dz} = 0 \Rightarrow N_{A,z} = c_2$$

$$N_{A,z} = \frac{c_A}{c}(N_{Az} + N_{Bz}) + J_{Az}^*$$

$$N_{Az} = x_A (N_{Az}) + J_{Az}^*$$

$N_{Az} - x_A N_{Az}$,

$N_{Az}(1-x_A)$

$$N_{Az} = \frac{1}{1-x_A} J_{Az}^*$$

$$= \underbrace{\frac{1}{1-x_A} cD_{AB}\frac{dx_A}{dz} = c_2}$$

(4-5) BC's & Math

$$\int \frac{1}{1-x_A}\, dx_A = \int \frac{c_2}{cD_{AB}}\, dz$$

$$-\ln(1-x_A) = \frac{c_2 z}{cD_{AB}} + c_3$$

+ BC's $\quad x_A(z_1) = x_{A1}, \quad x_A(z_2) = x_{A2}$

$$c_2 = -\ln K_2 \qquad c_3 = -\ln K_3$$

$$-\ln(1-x_A) = \frac{-(\ln K_2)\cdot z}{cD_{AB}} - \ln K_3$$

$$\alpha = \frac{z}{cD_{AB}} \qquad \alpha_1 = \frac{z_1}{cD_{AB}} \qquad \alpha_2 = \frac{z_2}{cD_{AB}}$$

$$-\ln(1-x_A) = -\ln K_2^{\alpha} - \ln K_3$$

$$-\ln(1-x_A) = -\ln(K_2^{\alpha} K_3)$$

$$\boxed{1-x_A = K_2^{\alpha} K_3}$$

Apply BC's

$$\rightarrow 1-x_{A1} = K_2^{\alpha_1} K_3$$

$$1-x_{A2} = K_2^{\alpha_2} K_3$$

$$\frac{1-x_{A1}}{1-x_{A2}} = \frac{K_2^{\alpha_1}}{K_2^{\alpha_2}} = K_2^{(\alpha_1-\alpha_2)} \rightarrow \frac{z_1-z_2}{cD_{AB}}$$

$$K_2 = \left(\frac{1-x_{A1}}{1-x_{A2}}\right)^{\frac{1}{\alpha_1-\alpha_2}}$$

$$1-x_{A1} = \left(\frac{1-x_{A1}}{1-x_{A2}}\right)^{\frac{\alpha_1}{\alpha_1-\alpha_2}} K_3$$

$$K_3 = (1-x_{A1})\left(\frac{1-x_{A1}}{1-x_{A2}}\right)^{\frac{-\alpha_1}{\alpha_1-\alpha_2}} = \frac{-z_1}{z_1-z_2}$$

$$1-x_A = K_2^{\alpha} K_3$$

$$= \left(\frac{1-x_{A1}}{1-x_{A2}}\right)^{\frac{\alpha}{\alpha_1-\alpha_2}} \cdot (1-x_{A1}) \left(\frac{1-x_{A1}}{1-x_{A2}}\right)^{\frac{-\alpha_1}{\alpha_1-\alpha_2}}$$

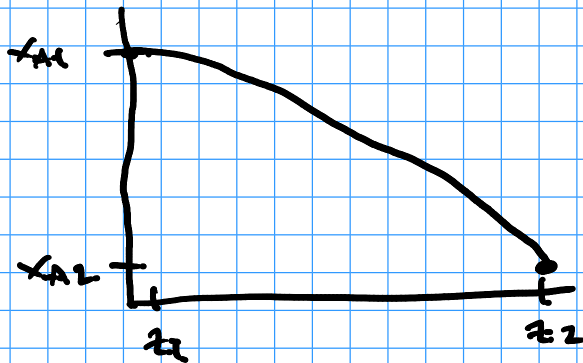
$$\frac{-\alpha_1}{\alpha_1-\alpha_2}$$

$$\frac{1-x_A}{1-x_{A1}} = \left(\frac{1-x_{A1}}{1-x_{A2}}\right)^{\frac{\alpha-\alpha_1}{\alpha_1-\alpha_2}}$$

$$\alpha = \frac{z}{CD_{AB}}$$

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

$x_B = 1 - x_A$ ✓



$$\underline{j} = \rho_A(\underline{v}_A - \underline{v})$$

$$\underline{v} - \underline{v}^{o}$$

$$- \underline{v}^{*}$$

IV. Chemical Reactions

* chem Rxn enters in 2 places

(1) A generation term (r_A, R_A).

This is a "homogeneous" chem rxn.

In bulk / in solution

(2) A boundary condition term.

This is a heterogeneous rxn.

At a surface.

For (1)

* you get things like this:

$$\frac{dN_{Az}}{dz} + f(c_A) = 0$$

$$\frac{d^2 c_A}{dz^2}$$

$\Rightarrow$ linear / non-linear 2nd order ODEs

Can't separate & integrate. §19.4

For (2): The boundary condition reflects the steady state flux

e.g. $A \rightarrow B$ $\quad N_{B,z}\big|_b = -N_{A,z}\big|_b$

$2A \rightarrow B$ $\quad N_{B,z}\big|_b = -\frac{1}{2} N_{A,z}\big|_b$

Ex. in § 18.3.

Shell Balance End!