17 April 2019 FAM ①

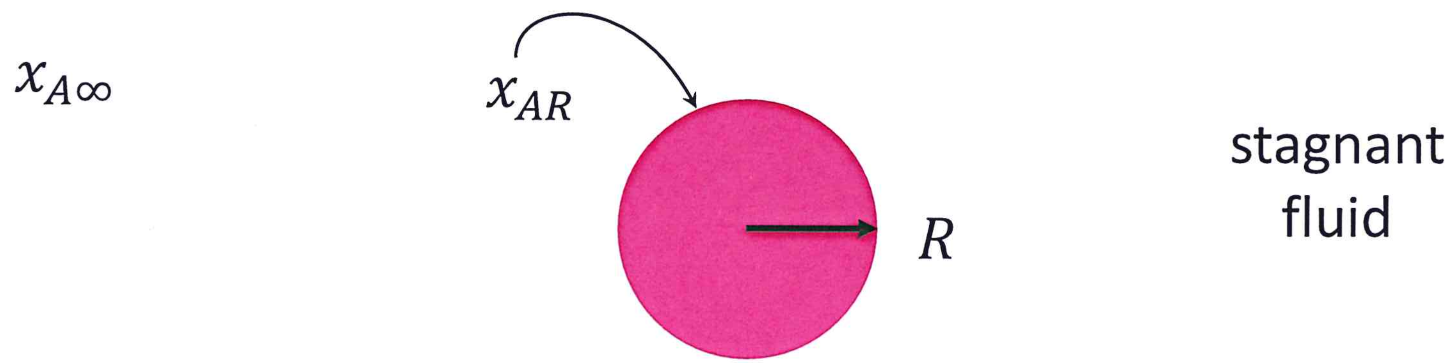
Routes to Mass Transfer Correlations

Theoretical

- Based on a model of the situation; can be solved for flux, and thus for k_x
- All models have assumptions; how good the assumptions are determine how good the correlations are
- The heat-transfer analogy counts as a theoretical pathway

mass

Example: A spherical medical pill dissolves slowly in a stagnant fluid (water). What is the mass transfer coefficient k_c? What is the Sherwood number for this situation?



Solve.

Which micro-species-A balance to use? This one in terms of x_A: 2

The **Equation of Species Mass Balance in Terms of Molar Quantities, constant cD_{AB}.** For binary systems, and Fick's law has been incorporated. Good for low density gases at constant temperature and pressure.

In terms of Diffusivity, D_{AB}

Microscopic species mass balance, constant thermal conductivity; Gibbs notation

$$c\left(\frac{\partial x_A}{\partial t} + \underline{v}^* \cdot \nabla x_A\right) = cD_{AB}\nabla^2 x_A + (x_B R_A - x_A R_B)$$

Microscopic species mass balance, constant thermal conductivity; Cartesian coordinates

$$c\left(\frac{\partial x_A}{\partial t} + v_x^*\frac{\partial x_A}{\partial x} + v_y^*\frac{\partial x_A}{\partial y} + v_z^*\frac{\partial x_A}{\partial z}\right) = cD_{AB}\left(\frac{\partial^2 x_A}{\partial x^2} + \frac{\partial^2 x_A}{\partial y^2} + \frac{\partial^2 x_A}{\partial z^2}\right) + (x_B R_A - x_A R_B)$$

Microscopic species mass balance, constant thermal conductivity; cylindrical coordinates

$$c\left(\frac{\partial x_A}{\partial t} + v_r^*\frac{\partial x_A}{\partial r} + \frac{v_\theta^*}{r}\frac{\partial x_A}{\partial \theta} + v_z^*\frac{\partial x_A}{\partial z}\right) = cD_{AB}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial x_A}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 x_A}{\partial \theta^2} + \frac{\partial^2 x_A}{\partial z^2}\right) + (x_B R_A - x_A R_B)$$

Microscopic species mass balance, constant thermal conductivity; spherical coordinates

$$c\left(\frac{\partial x_A}{\partial t} + \cancel{v_r^*\frac{\partial x_A}{\partial r}} + \cancel{\frac{v_\theta^*}{r}\frac{\partial x_A}{\partial \theta}} + \cancel{\frac{v_\phi^*}{r\sin\theta}\frac{\partial x_A}{\partial \phi}}\right)$$
$$= cD_{AB}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial x_A}{\partial r}\right) + \cancel{\frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial x_A}{\partial \theta}\right)} + \cancel{\frac{1}{r^2\sin^2\theta}\frac{\partial^2 x_A}{\partial \phi^2}}\right) + \cancel{(x_B R_A - x_A R_B)}$$

$cx_A = c_A = \frac{1}{M_A}(\rho_A) = \frac{1}{M_A}(\rho\omega_A)$ (units: $c[=]\frac{mol\ mix}{vol\ soln}$; $\rho[=]\frac{mass\ mix}{vol\ soln}$; $c_A[=]\frac{mol\ A}{vol\ soln}$; $\rho_A[=]\frac{mass\ A}{vol\ soln}$)

$v^* \neq 0$

$\underline{J}_A^* \equiv$ molar flux relative to a mixture's molar average velocity, $\underline{v}^*$ (units: $\underline{J}_A^*[=]\frac{mole}{area \cdot time}$)

$= c_A(\underline{v}_A - \underline{v}^*)$

$v^* \neq 0$ since diffusion is occurring...

$\underline{J}_A^* + \underline{J}_B^* = 0$

$\underline{N}_A \equiv c_A\underline{v}_A = \underline{J}_A^* + c_A\underline{v}^* =$ combined molar flux relative to stationary coordinates

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

$\underline{v}_A \equiv$ velocity of species A in a mixture, i.e. average velocity of all molecules of species A within a small volume

$\underline{v}^* = x_A\underline{v}_A + x_B\underline{v}_B \equiv$ molar average velocity

Reference: R. B. Bird, W. E. Stewart, and E. N. Lightfoot, *Transport Phenomena*, 2nd edition, Wiley, 2002. (p. 515, 584) try this version in terms of ω_A :

(3)

The **Equation of Species Mass Balance, constant ρD_{AB}.** For binary systems, and Fick's law has been incorporated. Good for dilute liquid solutions at constant temperature and pressure.

In terms of Diffusivity, D_{AB}

Microscopic species mass balance, constant thermal conductivity; Gibbs notation

$$\rho\left(\frac{\partial \omega_A}{\partial t} + \underline{v}\cdot\nabla\omega_A\right) = \rho D_{AB}\nabla^2\omega_A + r_A$$

Microscopic species mass balance, constant thermal conductivity; Cartesian coordinates

$$\rho\left(\frac{\partial \omega_A}{\partial t} + v_x\frac{\partial \omega_A}{\partial x} + v_y\frac{\partial \omega_A}{\partial y} + v_z\frac{\partial \omega_A}{\partial z}\right) = \rho D_{AB}\left(\frac{\partial^2\omega_A}{\partial x^2} + \frac{\partial^2\omega_A}{\partial y^2} + \frac{\partial^2\omega_A}{\partial z^2}\right) + r_A$$

Microscopic species mass balance, constant thermal conductivity; cylindrical coordinates

$$\rho\left(\frac{\partial \omega_A}{\partial t} + v_r\frac{\partial \omega_A}{\partial r} + \frac{v_\theta}{r}\frac{\partial \omega_A}{\partial \theta} + v_z\frac{\partial \omega_A}{\partial z}\right) = \rho D_{AB}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \omega_A}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2\omega_A}{\partial \theta^2} + \frac{\partial^2\omega_A}{\partial z^2}\right) + r_A$$

Microscopic species mass balance, constant thermal conductivity; spherical coordinates

ss

$$\rho\left(\cancel{\frac{\partial \omega_A}{\partial t}} + \cancel{v_r\frac{\partial \omega_A}{\partial r}} + \cancel{\frac{v_\theta}{r}\frac{\partial \omega_A}{\partial \theta}} + \cancel{\frac{v_\phi}{r\sin\theta}\frac{\partial \omega_A}{\partial \phi}}\right)$$
$$= \rho D_{AB}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial \omega_A}{\partial r}\right) + \cancel{\frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial \omega_A}{\partial \theta}\right)} + \cancel{\frac{1}{r^2\sin^2\theta}\frac{\partial^2\omega_A}{\partial \phi^2}}\right) + \cancel{r_A}$$

no homogeneous rxn

$\underline{v} = 0$ $\quad$ θ, ϕ symmetry

$cx_A = c_A = \frac{1}{M_A}(\rho_A) = \frac{1}{M_A}(\rho\omega_A)$ $\quad$ (units: $c[=]\frac{mol\ mix}{vol\ soln}$; $\rho[=]\frac{mass\ mix}{vol\ soln}$; $c_A[=]\frac{mol\ A}{vol\ soln}$; $\rho_A[=]\frac{mass\ A}{vol\ soln}$)

$\underline{j}_A \equiv$ mass flux of species A relative to a mixture's mass average velocity, $\underline{v}$ $\quad$ (units: $\underline{j}_A[=]\frac{mass\ A}{area\cdot time}$)

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

$\underline{j}_A + \underline{j}_B = 0$, i.e. these fluxes are measured relative to the mixture's center of mass

$\underline{n}_A \equiv \rho_A\underline{v}_A = \underline{j}_A + \rho_A\underline{v} =$ combined mass flux relative to stationary coordinates

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

$\underline{v}_A \equiv$ velocity of species A in a mixture, i.e. average velocity of all molecules of species A within a small volume

$\underline{v} = \omega_A\underline{v}_A + \omega_B\underline{v}_B \equiv$ mass average velocity; same velocity as in the microscopic momentum and energy balances

Reference: R. B. Bird, W. E. Stewart, and E. N. Lightfoot, *Transport Phenomena*, 2nd edition, Wiley, 2002.
(p. 515, 584)

Let's use the w_A one:

$$0 = \cancel{\rho}\, \cancel{D_{AB}}\, \cancel{\frac{1}{r^2}}\, \frac{d}{dr}\Big(\underbrace{r^2 \frac{dw_A}{dr}}_{\equiv \Phi}\Big)$$

$$\frac{d\Phi}{dr} = 0$$

$$\Phi = c_1 = r^2 \frac{dw_A}{dr}$$

$$\frac{dw_A}{dr} = \frac{c_1}{r^2}$$

$$\boxed{w_A = -\frac{c_1}{r} + c_2}$$

How can we convert w_A to x_A?

$$w_A = \frac{\text{mass } A}{\text{mass mix}} \qquad x_A = \frac{\text{mol } A}{\text{mol mix}}$$

$$= \frac{\text{mass } A}{\underbrace{\text{mass } A}_{\to 0 \text{ dilute}} + \text{mass } B} \qquad = \frac{\text{mol } A}{\underbrace{\text{mol } A}_{\to 0 \text{ dilute}} + \text{mol } B}$$

$$x_A = \frac{\cancel{\text{mass } A}}{\cancel{\text{mass } B}} \underbrace{\frac{\text{mol } A}{\cancel{\text{mass } A}}}_{\frac{1}{M_A}} \underbrace{\frac{\cancel{\text{mass } B}}{\text{mol } B}}_{M_B}$$

$$\boxed{x_A = w_A \frac{M_B}{M_A}}$$ (dilute mixture)

Let's convert the soln from WA to X_A: ⑥

$$\frac{M_B}{M_A} WA = \left(-\frac{c_1}{r} + c_2\right) \frac{M_B}{M_A}$$

$$\underbrace{X_A = -\frac{\tilde{c}_1}{r} + \tilde{c}_2}_{\text{Same as we would have gotten with the other version of the microscopic species A mass bal.}}$$

where:

$$c_1 \frac{M_B}{M_A} = \tilde{c}_1$$

$$c_2 \frac{M_B}{M_A} = \tilde{c}_2$$

Finish:

$$X_A = -\frac{\tilde{C}_1}{r} + \tilde{C}_2$$

BC: $r = \infty \quad X_A = X_{A\infty}$

$r = R \quad X_A = X_{AR}$

substituting: $X_{A\infty} = \tilde{C}_2$

$$X_{AR} = -\frac{\tilde{C}_1}{R} + C_2$$

$$\boxed{(X_{AR} - X_{A\infty})(-R) = \tilde{C}_1}$$

8

$$x_A = -\frac{1}{r}\left((-R)\left[x_{AR} - x_{A\infty}\right]\right) + x_{A\infty}$$

$$\boxed{x_A = \frac{R}{r}\left(x_{AR} - x_{A\infty}\right) + x_{A\infty}}$$

match fluxes at $r = R$:

$$k_x\left(x_{AR} - x_{A\infty}\right) = \underbrace{-c\, D_{AB} \overbrace{\frac{dx_A}{dr}}^{\tilde{c}_1/r^2}\bigg|_{r=R}}_{\text{from the reverse of the micro species A bal}}$$

$$k_x \cancel{(x_{AR} - x_{A\infty})} = \cancel{+} c D_{AB} \frac{(\cancel{+}\cancel{R}) \cancel{(x_{AR} - x_{A\infty})}}{R^{\cancel{2}}}$$

$$\boxed{k_x = \frac{c D_{AB}}{R}}$$

$$Sh = \frac{D k_x}{c D_{AB}} \qquad (D = 2R)$$

$$= 2\cancel{R} \frac{\cancel{c D_{AB}}}{\cancel{R}} \frac{1}{\cancel{c D_{AB}}}$$

$$\boxed{Sh = 2}$$

// Heat - Mass analogy holds.