MODULE 4 LEC XIII 19 April 2021 CM3120 F. Morrison 1

Theoretical Pathway to Mass Transfer Coefficients:

The Heat/Mass Transfer Analogy

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?

heat

Example: A spherical pellet of reacting solid slowly emits heats steadily into a stagnant fluid such that the surface temperature is constant. What is the heat transfer coefficient h? What is the Nusselt number for this situation?

BSL2 p321, problem 10B.1, p678

HEAT XFER

The Heat/Mass Transfer Analogy

heat

Example 16: A spherical pellet of reacting solid slowly emits heats steadily into a stagnant fluid such that the surface temperature is constant. What is the heat transfer coefficient h? What is the Nusselt number for this situation?

Routes to Mass Transfer Correlations

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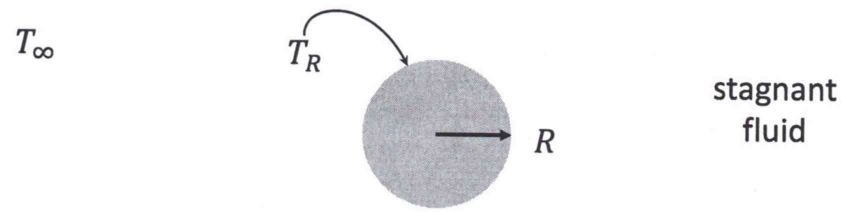

Solve.

Let's "slash them" both

BSL2 p321, problem 10B.1

MASS XFER

The Heat/Mass Transfer Analogy

mass

Example 17: 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?

Routes to Mass Transfer Correlations

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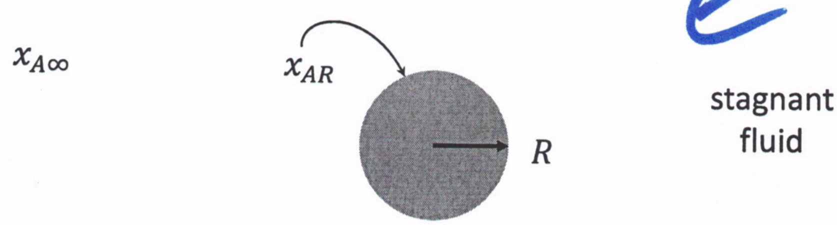

Solve.

BSL2 p321, problem 10B.1

★ HEAT

Domain $R \le r < \infty$ (fluid)

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The **Equation of Energy** for systems with **constant k**

Microscopic energy balance, constant thermal conductivity; Gibbs notation

$$\rho \hat{C}_p \left(\frac{\partial T}{\partial t} + \underline{v} \cdot \nabla T \right) = k \nabla^2 T + S_e$$

Microscopic energy balance, constant thermal conductivity; Cartesian coordinates

$$\rho \hat{C}_p \left(\frac{\partial T}{\partial t} + v_x \frac{\partial T}{\partial x} + v_y \frac{\partial T}{\partial y} + v_z \frac{\partial T}{\partial z} \right) = k \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) + S_e$$

Microscopic energy balance, constant thermal conductivity; cylindrical coordinates

$$\rho \hat{C}_p \left(\frac{\partial T}{\partial t} + v_r \frac{\partial T}{\partial r} + \frac{v_\theta}{r} \frac{\partial T}{\partial \theta} + v_z \frac{\partial T}{\partial z} \right) = k \left(\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 T}{\partial \theta^2} + \frac{\partial^2 T}{\partial z^2} \right) + S_e$$

steady   stagnant fluid $\underline{v} = 0$

Microscopic energy balance, constant thermal conductivity; spherical coordinates

$$\rho \hat{C}_p \left(\cancel{\frac{\partial T}{\partial t}} + \cancel{v_r \frac{\partial T}{\partial r}} + \cancel{\frac{v_\theta}{r} \frac{\partial T}{\partial \theta}} + \cancel{\frac{v_\phi}{r \sin\theta} \frac{\partial T}{\partial \phi}} \right)$$
$$= k \left(\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial T}{\partial r} \right) + \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \cancel{\frac{\partial T}{\partial \theta}} \right) + \frac{1}{r^2 \sin^2\theta} \cancel{\frac{\partial^2 T}{\partial \phi^2}} \right) + \cancel{S_e}$$

1D radial

no elect current, no rxn

$$0 = \cancel{\frac{k}{r^2}} \frac{d}{dr} \underbrace{\left(r^2 \frac{dT}{dr} \right)}_{\equiv \Phi}$$

$$\frac{d\Phi}{dr} = 0 \qquad \Phi = C_1 = r^2 \frac{dT}{dr}$$

$$\frac{dT}{dr} = \frac{C_1}{r^2}$$

Reference: F. A. Morrison, "Web Appendix to *An Introduction to Fluid Mechanics*," Cambridge University Press, New York, 2013 (*pages.mtu.edu/~fmorriso/cm310/IFMWebAppendixDMicroEBalanceMorrison.pdf*). This worksheet is on the web at *pages.mtu.edu/~fmorriso/cm310/energy.pdf*.

$$T = -\frac{C_1}{r} + C_2$$

BC $\quad r = R \quad T = T_R$

$\quad\quad r = \infty \quad T = T_\infty$

HEAT

solve for c_1, c_2

$$T = -\frac{c_1}{r} + c_2$$

$$T_R = -\frac{c_1}{R} + c_2$$

$$\boxed{T_\infty = c_2}$$

$$\boxed{-R(T_R - T_\infty) = c_1}$$

$$\boxed{T = \frac{R}{r}(T_R - T_\infty) + T_\infty}$$

check BC: $r=R$ $T=T_R$
$r\to\infty$ $T=T_\infty$ ✓

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What is Nu?

at $r = R$:

$$-k \underbrace{\frac{dT}{dr}}_{\text{use } T(r)} = h(T - T_\infty)$$

$$+k \left.\frac{\cancel{R}\,\cancel{(T_R - T_\infty)}}{r^2}\right|_{r=R} = h\,\cancel{(T_R - T_\infty)}$$

$r^2 = R^2$

$$Nu = \frac{hD}{k} = \frac{2Rh}{k} = \frac{2\cancel{R}}{\cancel{k}}\,\frac{\cancel{k}}{\cancel{R}} = 2 \qquad \boxed{Nu = 2}$$

MASS (pmph) Domain $R \le r < \infty$ 6

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

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

stdy stagnant fluid $\underline{v} = 0$

Microscopic species mass balance, constant thermal conductivity; spherical coordinates

$$\rho\left(\cancel{\frac{\partial \omega_A}{\partial t}} + \cancel{v_r\frac{\partial \omega_A}{\partial r}} + \cancel{\frac{v_\theta}{r}\frac{\partial \omega_A}{\partial \theta}} + \cancel{\frac{v_\phi}{r\sin\theta}\frac{\partial \omega_A}{\partial \phi}}\right)$$

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

1D radial

no homogeneous rxn

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

$\underline{j}_A \equiv$ mass flux of species A relative to a mixture's mass average velocity, $\underline{v}$ (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

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

$$0 = \cancel{\rho}\,\cancel{D_{AB}}\,\cancel{\frac{1}{r^2}}\frac{d}{dr}\left(r^2\frac{d\omega_A}{dr}\right)$$

$\underline{v}_A \equiv$ 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

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

MASS solve for species A distribution w/ r

$$0 = \frac{d}{dr}\Big(\underbrace{r^2 \frac{dw_A}{dr}}_{\equiv \Phi}\Big)$$

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

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

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

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

BC: $r = R$ $w_A = w_{AR}$

$r = \infty$ $w_A = w_{A\infty}$

same math plm as last case (p3)

Note: molar units are more common. Let's switch to molar units

$$w_A = \frac{\text{mass } A}{\text{mass total}}$$

$$\Bigg(\frac{\cancel{\text{mass}}\,A}{\underbrace{\text{mass total}}_{\text{mass}A \,+\, \cancel{\text{mass } B}}}\Bigg)\Bigg(\underbrace{\frac{\text{mol } A}{\cancel{\text{mass } A}}}_{\frac{1}{M_A}}\Bigg)\Bigg(\underbrace{\frac{\cancel{\text{mass}}\ B}{\text{mol } B}}_{M_B}\Bigg)$$

assum dilute

$$X_A = w_A \frac{1}{M_A} M_B \quad \text{(dilute mixture)}$$

$$\boxed{w_A = \frac{M_A}{M_B} X_A \;\Big|\; \text{(dilute)}}$$

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

$$\frac{M_A}{M_B} x_A = \frac{-c_1}{r} + c_2$$

$$x_A = -\underbrace{\left(\frac{c_1 M_B}{M_A}\right)}_{\tilde{c}_1} \frac{1}{r} + \underbrace{\frac{c_2 M_B}{M_A}}_{\tilde{c}_2}$$

$$x_A = \frac{-\tilde{c}_1}{r} + \tilde{c}_2$$

(Same eqn since we have yet to apply BC)

(transform BC too)

Apply BC

Algebra

Soln:

DILUTE MIX

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

(same soln as for heat, mathematically)

from this at r=R

What is Sh?

at r=R

film coef

in LiQ, at r=R:

$$\underbrace{-cD_{AB}\frac{\partial x_A}{\partial r}}_{\text{Fick's Law}} = \underbrace{k_x\left(x_{AR} - x_{A\infty}\right)}_{\text{linear driving force model}}$$

$$\frac{\partial x_A}{\partial r} = \frac{-R\left(x_{AR} - x_{A\infty}\right)}{r^2}$$

$$\left.\frac{\partial x_A}{\partial r}\right|_{r=R} = \frac{-\left(x_{AR} - x_{A\infty}\right)}{R}$$

combine:

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

diameter

DILUTE MIX

$$\boxed{2 = \frac{k_x D}{c\,D_{AB}} = Sh}$$

Analogous to heat xfer case (Nu = 2 also!)