CHE 318 Lecture 15

Theories For Mass Transfer Coefficients

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Learning Outcomes

After today's lecture, you will be able to:

- Recall theoretical models for mass transfer coefficients
- Understand the "interface thickness" associated with mass transfer
- Analyze different power laws associated with D_{AB} to k'_c

Example 1: Convective Flux Through A Tube

Question: Consider steady-state, one-dimensional mass transfer of a binary gas mixture consisting of species A and B between two parallel planes, labeled (1) and (2). The total pressure of the system is $p_T = 700$ kPa and the temperature is maintained at $T = 100$°C. The gas-phase mass transfer coefficient from molar fraction is $k_y' = 1.5 \times 10^{-4}$ kg mol $\cdot$ m^{-2} $\cdot$ s^{-1}. Flow in pipe 1 contains 65 mol% A, while flow in pipe 2 contains 45 mol% B.

1. Find the values for fluxes N_A and N_B
2. Find the values (and units) for other coefficients k'_G and k'_c

Solutions To Example 1

> **Tip**
>
> - Mass transport normal to fluid can usually use k to write the flux equation
> - Pay attention to the unit used

Answer

1. $N_A = -N_B = 3.0 \times 10^{-5}$ kg mol $\cdot$ m^{-2} $\cdot$ s^{-1}

2. $k'_G = k'_y/p_T = 2.14 \times 10^{-7}$ kg mol/(m$^2 \cdot$ s $\cdot\, kPa$)
3. $k'_c = k'_y RT/p_T = 6.65 \times 10^{-4}$ m $\cdot$ s^{-1}

Example 2: Using k For Diffusion Through Stagnant Film

Geankoplis Ex 7.2-1 A large volume of pure gas B at 2 atm pressure flows over a flat surface. Species A is vaporizing from the surface into the gas stream. The liquid A completely wets the surface of a blotting paper, so that the interface is always covered with liquid A. The partial pressure of species A at 298 K is 0.20 atm. From textbook table,

$$k'_y = 6.78 \times 10^{-5}\ \frac{\text{kg mol}}{\text{m}^2 \cdot \text{s}}$$

.

Calculate the evaporation rate N_A and determine the values of the gas-phase mass transfer coefficients k_y and k_G for this system.

Solutions To Example 2

Tip

- This is a diffusion through stagnant B system
- Convert k'_y to k_y in stagnant B system first
- Express k_G in kg mol/(s $\cdot$ m^2 $\cdot$ atm) first

Answer

1. $y_{Bm} = 0.95 \quad k_y = k'_y/y_{Bm} = 7.138 \times 10^{-5}\ \frac{\text{kg mol}}{\text{m}^2\cdot\text{s}}$
2. $y_G = 3.569 \times 10^{-5}$ kg mol/(s $\cdot$ m^2 $\cdot$ atm)
3. $N_A = y_G(p_{A1} - p_{A2}) = 7.138 \times 10^{-6}$ kg mol $\cdot$ m^{-2} $\cdot$ s^{-1}

Example 3: Measuring k For Actual Systems

Since we have [Flux] = k × [Driving Force], we can measure k using given geometries.

Question: solid benzoic acid (A) in a sphere with radius r_0 was place in a tube with water flowing in the system. The fluid was turned on for a certain time interval Δt to remove dissolved A from the liquid. The masses of a dried sphere before and after the experiment were measured to be m_1 and m_2 ($m_2 - m_1 \ll m_1$). The solubility of A in water is c_{As} and water contain no benzoid acid. Calculate the mass transfer coefficient of this system. What form of k did you use?

Solutions To Example 3

Tip

- Flow-induced flux, can be turbulent lumped k_L term is valid
- Link N_A to mass loss rate

Answer:

- Relating flux equation to mass loss rate:

$$
\begin{aligned}
N_A &= \frac{1}{4\pi r_0^2} \frac{m_1 - m_2}{M_A \Delta t} && (1) \\
&= k_L (c_{As} - 0) && (2)
\end{aligned}
$$

- Solve for k_L:

$$
k_L = \frac{1}{4\pi r_0^2} \frac{m_1 - m_2}{c_{As} M_A \Delta t} \tag{3}
$$

How Can We Predict The k_c' Values?

- k_c' is a convenient parameter, but is system dependent!
- $k_c' = f(D_{AB}, v_m, \mu, \rho, T, [\text{Geometry}]), ...$
- Several theories attemp to build the form of such relation:

  1. Film mass transfer theory
  2. Penetration theory
  3. Boundary layer theory

- Different forms & applicable scenarios

Film Mass Transfer Theory

- Nernst (1904) & Whitman (1923), based on convective heat transfer
- Assumptions:

  1. A thin layer with thickness δ_f exists at the boundary of the interface
  2. Only **diffusive mass transfer** occur in the film
  3. Convection occurs **outside** the film region

Film Mass Transfer Theory: Equations

Inside the thin film region, we have EMCD-like mass transfer

$$
\begin{aligned}
N_A &= J^*_{Az} &(4)\\
&= -D_{AB}\frac{dc_A}{dz} &(5)\\
&= \boxed{\frac{D_{AB}}{\delta_f}}(c_{A,i} - c_{A,b}) &(6)\\
&= k'_c(c_{A,i} - c_{A,b}) &(7)
\end{aligned}
$$

- Predicts $k'_c \propto D_{AB}^{1.0}$ (Incorrect in most cases)
- Simple prediction of k'_c if we know δ_f
- δ_f is linked to both D_{AB} and ϵ_m

Penetration Theory

- Higbie (1935) & Danckwerts (1950) for gas-liquid interface
- Assumptions:
  1. Gas molecules penetrate into laminar film surrounding the interface
  2. The penetration time is usually very short
  3. Fluid makes contact with the gas molecules and return to the bulk
  4. The penetration process can be modeled by time-dependent unsteady state mass transfer!

Penetration Theory: Equations

- Governing equation for mass transfer (no convection in the film)

$$
\frac{\partial c_A}{\partial t} = D_{AB}\frac{\partial^2 c_A}{\partial z^2} \tag{8}
$$

- B.C. $c_A(z=0) = c_{A,s},\ c_A(z=\infty) = c_{A,b}$

Penetration Theory: Solutions

The concentration inside the liquid film has the following solution:

$$\frac{c_A(z,t) - c_{A,b}}{c_{A,s} - c_{A,b}} = 1 - \text{erf}\left(\frac{z}{\sqrt{4D_{AB}t}}\right) \tag{9}$$

We can directly get N_A from $\frac{\partial c_A}{\partial z}|_{\text{surf}}$:

$$N_A(z=0,t) = -D_{AB}\frac{dc_A}{dt} \tag{10}$$

$$= \sqrt{\frac{D_{AB}}{\pi t}}(c_{A,s} - c_{A,b}) \tag{11}$$

Penetration Theory: Power Law

We can calculate the average N_A in the penetration period ($0 < t < t_L$):

$$N_A = \frac{1}{t_L}\int_0^{t_L} -D_{AB}\frac{dc_A}{dt'} \tag{12}$$

$$= \boxed{\sqrt{\frac{4D_{AB}}{\pi t_L}}}(c_{A,s} - c_{A,b}) \tag{13}$$

$$= k'_c(c_{A,s} - c_{A,b}) \tag{14}$$

- Penetration theory predicts $k'_c \propto D_{AB}^{0.5}$
- Practical power law $k'_c \propto D_{AB}^n;\ n = 0.8 \sim 0.9$
- Danckwert's renewal model: $k'_c \propto (D_{AB}s)^{0.5}$ correction to power law using s

Boundary Layer Theory

- Theory connecting fluid dynamics ($v_m = [v_x, v_y]$) and mass transfer coefficient
- Fluid velocity field associate with a boundary thickness δ
- Conversely the concentration in fluid has a boundary δ_c
- Boundary layer theory solves c_A profile using analogs in momentum transfer

Boundary Layer Theory: Equations

The mass balance equation for a steady-state 2D problem without generation

$$-\nabla \cdot \vec{N}_A = 0 \tag{15}$$
$$-\nabla \cdot (\vec{J}_A^* + c_A \vec{v}) = 0 \tag{16}$$
$$\vec{v} \cdot \nabla c_A = D_{AB} \nabla^2 c_A \tag{17}$$
$$v_x \frac{\partial c_A}{\partial x} + v_y \frac{\partial c_A}{\partial y} = D_{AB} \frac{\partial^2 c_A}{\partial y^2} \tag{18}$$

- Mass transfer in x-direction (fluid direction) is convective
- Diffusive contribution only occur in y-direction (normal to fluid)
- Boundary conditions:
  - $y = 0$ (on surface) $\frac{v_x}{v_b} = (c_A - c_{A,s})/(c_{A,b} - c_{A,s}) = 0$
  - $y = \infty$ (center of fluid) $\frac{v_x}{v_b} = (c_A - c_{A,s})/(c_{A,b} - c_{A,s}) = 1$

Boundary Layer Theory: Concentration Profile

If the boundary thickness for fluid δ and concentration δ_c are same, can use the solution to velocity field:

$$\left(\frac{\partial c_A}{\partial y}\right)_{y=0} = (c_{A,\infty} - c_{A,s}) \left(\frac{0.332}{x} N_{Re,x}^{0.5}\right) \tag{19}$$

- Here $N_{Re,x} = xv\rho/\mu$ is the location-dependent Reynolds number (to be discussed later)
- Because $\partial c_A/\partial y$ is known –> we can get the expression for k_c'!

Boundary Layer Theory: Final Results

Boundary layer theory links diffusion in y-direction with:

$$N_{Ay} = k_c'(c_{A,s} - c_{A,b}) \tag{20}$$
$$= \boxed{-D_{AB} \left(\frac{0.332}{x} N_{Re,x}^{0.5}\right)} (c_{A,\infty} - c_{A,s}) \tag{21}$$

For $\delta = \delta_c$, we have k_c' expression:

$$k_c' = \frac{0.332 D_{AB}}{x} N_{Re,x}^{0.5} \tag{22}$$

Generally, we have Schmidt number $N_{Sc} = (\delta/\delta_c)^3$, so

$$k_c' = \frac{0.332 D_{AB}}{x} N_{Re,x}^{0.5} N_{Sc}^{1/3} \tag{23}$$

The global mass transfer coefficient should integrate over $0 \sim L$:

$$k_c' = \frac{0.664 D_{AB}}{L} N_{Re}^{0.5} N_{Sc}^{1/3} \tag{24}$$

- where $N_{Re} = (\rho L v)/\mu$ is the overall Reynolds number
- boundary layer theory predicts $k_c' \propto D_{AB}^{2/3}$ (as $N_{Sc} \propto 1/D_{AB}$)

Comparison Between Theories For k_c'

Approach	Governing expression for N_A	Scaling of k_c' with D_{AB}
Film theory	$N_A = \frac{D_{AB}}{\delta}(c_{A,s} - c_{A,b})$	$k_c' \propto D_{AB}$
Penetration theory	$N_A = \sqrt{\frac{4D_{AB}}{\pi t_L}}(c_{A,s} - c_{A,b})$	$k_c' \propto D_{AB}^{0.5}$
Boundary layer theory	$N_A = 0.664\, D_{AB}/L\, N_{Sc}^{1/3}\, N_{Re}^{1/2}(c_{As} - c_{A,b})$	$k_c' \propto D_{AB}^{2/3}$
General formula	–	$k_c' \propto D_{AB}^n n = 0.5 \sim 0.9$

Summary

In this lecture, we showed a few theories that can elucidate the physics behind k_c', mostly relating to D_{AB} by different boundary conditions

- Thin film theory: physically intuitive, hard to estimate film thickness
- Penetration theory: capturing dynamic behaviour of gas-liquid exchange
- Boundary layer theory: most accurate, requiring usage of dimensionless numbers

Why do we need dimensionless numbers? We will see in the next lecture.