CHE 318 Lecture 14

Mass Transfer Coefficients (II)

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Recap

- Introduction to mass transfer coefficients
- Link between mass transfer coefficient and diffusivity
- Introduction to boundary concentration problem

Learning Outcomes

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

- Remember the flux equations using mass transfer coefficient in different phases
- Recall the motivation of using mass transfer coefficient
- Analyze mass transfer coefficients' units
- Distinguish between mass transfer coefficients in different forms

Realistic Interfacial Concentration Profiles

At the boundary, it is often convenient to use the equilibrium concentration ratio between gas (c_i) and liquid (c_{Li}). This constant, often called the **equilibrium distribution coefficient**, is defined as:

$$K = \frac{\text{[Conc. at gas side]}}{\text{[Conc. at liquid side]}} \tag{1}$$

$$= \frac{c_i}{c_{Li}} \tag{2}$$

- Similarity: Henry's law ($H = \frac{p_{\text{gas}}}{c_{\text{aq}}}$), remember in gas $p_{\text{gas}} = c_{\text{gas}}RT$

- We have already seen similar concepts in solubility in liquid / solid diffusion equations!
- K can be a value range from 0 to ∞ what does that mean?

Interfacial Concentration Profile For Different K

- The interfacial concentration values depend on the value of K!
- What else determines the interfacial balance? matching of interfacial fluxes N_A at both sides!

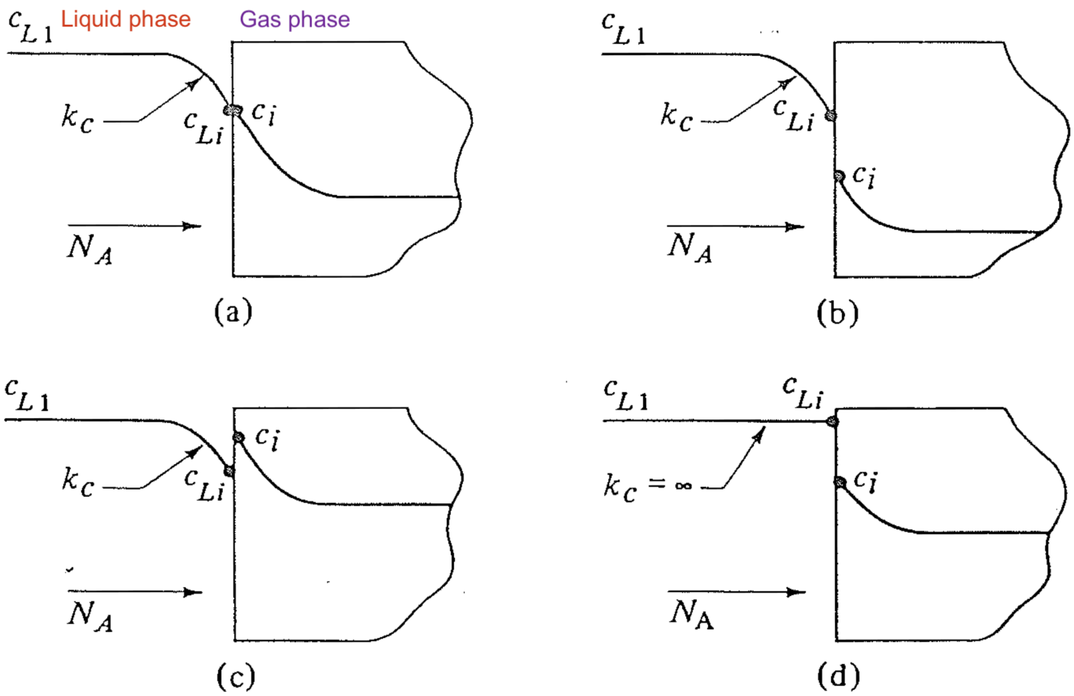

Figure 1: *Geankoplis Figure 7.1.3*

Match of Interfacial Fluxes

At equilibrium, if there is no resistance when transferring A between the interface, what is the mass balance equation?

$$[\text{In}]|_{\text{left}} - [\text{Out}]|_{\text{right}} + [\text{Gen}]|_{\text{interface}} = [\text{Acc}]|_{\text{interface}} \quad (3)$$

$$N_A|_{\text{left}} = N_A|_{\text{right}} \quad (4)$$

How do we model N_A in each phase?

- May be a combination of diffusion and convection
- Fluid velocity at interface may be turbulent (hard to model)
- In general we use the phenomenal relation [Flux] = [Driving Force]/[Resistance]

General Flux Equation For Convective Transport Regime

- The driving force is the concentration difference "bulk concentration" and "interfacial concentration"
- The resistance is lumped into one coefficient k'_c, **mass transfer coefficient**.

$$N_A = k'_c(c_{L,b} - c_{Li}) \tag{5}$$

- k'_c is inversely related to the resistance.
- k'_c means driving force is concentration & convection term is EMCD-like
- The unit of k'_c? $\quad \mathrm{m \cdot s^{-1}}$
- k'_c can be ∞! No transfer resistance inside the bulk phase

Where Does k'_c Come From (I)?

Simplified view: transport resistance of A from bulk to the interface occurs inside an interfacial film with thickness δ. We can write N_A at steady state using already known results

- Case 1: EMCD / diffusion-controlled / dilute transport in liquid

$$N_A = \boxed{\frac{D_{AB}}{\delta}}(c_{L,b} - c_{L,i}) \tag{6}$$

$$= k'_c(c_{L,b} - c_{L,i}) \tag{7}$$

- Case 2: transport in stagnant film with non-negligible convection

$$N_A = \boxed{\frac{D_{AB}}{\delta(1 - \frac{c}{c_T})}}(c_{L,b} - c_{L,i}) \tag{8}$$

$$= k'_c \frac{1}{x_{Bm}}(c_{L,b} - c_{L,i}) \tag{9}$$

$$= k_c(c_{L,b} - c_{L,i}) \tag{10}$$

- Can be written both by k'_c or k_c terms
- One can expect k_c contain the $1/x_{Bm}$ term!

Where Does k_c Come From (II)?

The mass transfer coefficient k_c is even valid for systems with effective D_{AB}!

- Case 3: mass transfer in porous solid materials

$$N_A = \boxed{\frac{\epsilon}{\tau}\frac{D_{AB}}{\delta}}(c_{L,b} - c_{L,i}) \tag{11}$$

$$= k_c'(c_{L,b} - c_{L,i}) \tag{12}$$

- Case 4: turbulent mass transfer

The turbulence in the fluid contributes to an additional term ϵ_m in diffusion terms

$$N_A = \boxed{\frac{D_{AB} + \epsilon_m}{\delta}}(c_{L,b} - c_{L,i}) \tag{13}$$

$$= k_c'(c_{L,b} - c_{L,i}) \tag{14}$$

- ϵ_m is the "Eddie diffusivity" (correction to D_{AB} due to turbulence)
- General case for ϵ_m is non-trivial to solve!

Implications of Mass Transfer Coefficient k_c'

- Really convenient to use!
- In reality, k_c' is not a physics-based quantity, it depends on system / condition
- $k_c' \propto D_{AB}^n$ in realistic systems
- We will discuss about different theories that explains the relation between k_c' and D_{AB} (penetration theory, film theory, boundary theory) in coming weeks

Balance Equations At Interfaces

We now have 2 equations to determine the interfacial concentrations!

1. Equilibrium concentration distribution

$$K = \frac{c_{g,i}}{c_{L,i}} \tag{15}$$

2. Flux matching

$$N_A|_{\text{liq}} = N_A|_{\text{gas}} \tag{16}$$

$$k'_{c,\text{liq}}(c_{L,b} - c_{L,i}) = k'_{c,\text{gas}}(c_{g,i} - c_{g,b}) \tag{17}$$

We can solve $c_{L,i}$ and $c_{g,i}$ given information about:

- Bulk concentrations $c_{L,b}$, $c_{g,b}$
- Equilibrium distribution coefficient K
- Mass transfer coefficients k_c in each phase

Demonstration of Mixed Boundary Conditions

Mass Transfer Coefficient In Different Forms

When using k to express flux, we have the **same form** (*Geankoplis Table 7.2.1*)

- Flux equations for EMCD

$$\text{Gases:} \quad N_A = k'_c\,(c_{A1} - c_{A2}) = k'_G\,(p_{A1} - p_{A2}) = k'_y\,(y_{A1} - y_{A2}) \tag{18}$$

$$\text{Liquids:} \quad N_A = k'_c\,(c_{A1} - c_{A2}) = k'_L\,(c_{A1} - c_{A2}) = k'_x\,(x_{A1} - x_{A2}) \tag{19}$$

- Flux equations for diffusion through stagnant B

$$\text{Gases:} \quad N_A = k_c\,(c_{A1} - c_{A2}) = k_G\,(p_{A1} - p_{A2}) = k_y\,(y_{A1} - y_{A2}) \tag{20}$$

$$\text{Liquids:} \quad N_A = k_c\,(c_{A1} - c_{A2}) = k_L\,(c_{A1} - c_{A2}) = k_x\,(x_{A1} - x_{A2}) \tag{21}$$

But:

- k'_c and k_c are two different coefficients
- k'_c, k'_L, k'_G have different units

Naming Convention and Units

- Superscript: EMCD $k'_{\text{driving force}}$; Convective / stagnant B $k_{\text{driving force}}$

Phase / Driving force	Concentration c_A	Partial pressure p_A	Mole fraction(gas y_A, liquid x_A)
Gas phase	k_c, k'_c	k_G, k'_G	k_y, k'_y
Liquid phase	k_c, k'_c	–	k_x, k'_x
Liquid (alt. form)	k_L, k'_L	–	–
Unit of k	$\mathrm{m \cdot s^{-1}}$	$\dfrac{\text{kg mol}}{\mathrm{s \cdot m^2 \cdot Pa}}$	$\dfrac{\text{kg mol}}{\mathrm{s \cdot m^2} \cdot \text{mol frac}}$

Conversions Between Mass Transfer Coefficients

Gas phase

$$k'_c\, c_T = k'_c \frac{p_T}{RT} = k_c \frac{p_{Bm}}{RT} \tag{22}$$

$$= k'_G\, p_T = k_G\, p_{Bm} \tag{23}$$

$$= k'_y = k_y\, y_{Bm} \tag{24}$$

$$= k_c\, y_{Bm}\, c_T = k_G\, y_{Bm}\, p_T \tag{25}$$

- $p:$ total pressure
- $p_{Bm}:$ log-mean partial pressure of inert B
- $y_{Bm}:$ log-mean mole fraction of B
- $c_T = p_T/(RT)$

Liquid phase

$$k'_c\, c = k'_L\, c = k_L\, x_{Bm}\, c \tag{26}$$

$$= k'_L\, \frac{\rho}{M} = k'_x = k_x\, x_{Bm} \tag{27}$$

- $\rho:$ liquid density
- $M:$ molecular weight
- $x_{Bm}:$ log-mean mole fraction of solvent B

Summary

In this lecture, we talked about

- The difficulty of studying boundary problems in mass transfer
- The rise of equilibrium distribution coefficient K and mass transfer coefficient k
- Link between mass transfer coefficient k and transfer layer

What To Learn Next

The concept of mass transfer coefficient k is both beautiful and ugly.

- We **gain** the simplicity of expressing flux equations using simple formula,
- We **lose** physical understanding about its origin in many systems

In next lectures, we will see:

- How to use mass transfer coefficients for different phases (gas, liquid, solid)
- How convective fluid transport is expressed using coefficients
- How to perform mass transfer analysis based on transfer coefficients