Interphase mass transfer III: Applications

Flux to concentration change (in water)

$$J_{tot} = -K_L (C_{bulk}{}^L - C_{bulk}{}^{L*})$$

Flux rate per unit area

$$A \cdot J_{tot} = -K_L \cdot A(C_{bulk}{}^L - C_{bulk}{}^{L*})$$

Total flux (A is area of air-water interface)

$$\frac{dC_{bulk}^{L}}{dt} = \left(\frac{A}{V}\right) J_{tot} = -K_L \left(\frac{A}{V}\right) \left(C_{bulk}^{L} - C_{bulk}^{L*}\right) = -K_L a \left(C_{bulk}^{L} - C_{bulk}^{L*}\right)$$

This is the rate of change in concentration in water

a = interfacial area for mass transfer per unit volume, A/V [L⁻¹] V = volume in which concentration is changing [L³] K_La = volumetric mass transfer coefficient [T⁻¹]

Mass transfer example: change in stream DO

Studies of **oxygen reaeration in streams** have been reasonably fit by the following (O'Connor & Dobbins, 1958)*:

$$K_L = \left(\frac{D_L u}{H}\right)^{0.5} = k_L$$

$$K_L a = \frac{(D_L u)^{0.5}}{H^{1.5}}$$

u = stream velocity, m/s H = 1/a = average stream depth, m D_L = liquid phase diffusivity, m²/s

* Connor, D. J., Dobbins, W. E. (1958) Mechanism of reaeration in natural systems. Transactions of the American Society of Civil Engineers, 23(1): 641-666.

Mass transfer example: change in stream DO

• Applying surface renewal model:

O'Connor and Dobbins hypothesized that

$$s_L = \frac{Avg.vertical velocity by turbulence}{Avg.mixing length} = \frac{0.1u}{0.1H} = \frac{u}{H}$$

Therefore,

$$K_L \approx k_L = (D_L s_L)^{1/2} = \left(\frac{D_L u}{H}\right)^{1/2}$$

Mass transfer example: change in stream DO

• Applying boundary layer theory:

$$k_L = \frac{(Sh)_L D_L}{d} = \frac{a_2 (Re)^{a_3} (v)^{a_4} D_L^{1-a_4}}{d} = a_2 d^{(a_3-1)} u^{a_3} v^{(a_4-a_3)} D_L^{(1-a_4)}$$

If
$$a_2 = 1.0$$
; $a_3 \& a_4 = 0.5$:

$$K_L \approx k_L = \left(\frac{D_L u}{d}\right)^{0.5}$$

Boundary layer theory: applications

Transfer to particle surface in stagnant fluid:

$$\frac{k_L d}{D_L} (Sh)_L = a_1 + a_2 (Re)^{a_3} (Sc)_L^{a_4}$$

$R_{\rho} = \frac{d \times u}{d - d}$	$d \times u \times \rho$	
v = v	μ	
$(Sc)_L^{a_4} = \frac{\nu}{D_L}$	$=\frac{\mu}{D_L\rho}$	

Here, $a_1 = 2$ $k_L = \frac{2D_L}{d_p} = \frac{D_L}{r_p} \approx \frac{1 \times 10^{-9}}{r_p} m/sec$ $a = \frac{area}{volume} = \frac{6}{d_p} m^{-1}$

If resistance is dominant at liquid phase,

$$K_L a \approx k_L a \approx \frac{10^{-8}}{d_p^2} \ sec^{-1}$$

Equilibration time can be characterized by $1/k_{L}a$

Wind effects on mass transfer



Mass transfer summary

• Molecular diffusion important over short lengths

- Thin, stagnant regions at interphases
- Turbulence critical at macroscopic levels
 - Mixing within phase
 - Generating interfacial surfaces

• Three models

- Differing versions of the interfacial region
 - Difficult/impossible to directly measure region
 - Infer interfacial region properties from experimental data
 - Models differ in molecular diffusion's impact on overall mass transfer
- For many compounds mass transfer resistance in one phase controls overall mass transfer rate

Interphase mass transfer IV: Exercise

Controlling resistance

Q: You set an experiment to determine the overall mass transfer coefficient with liquid phase as a reference, K_L , for gas-liquid transfer of oxygen and ethanol in a well-mixed reactor. You also need to estimate the K_L for nitrogen, which was not determined by the experiment. The results of the experiment, the Henry's law constants, and the diffusion coefficients in water are as follows:

Compounds	K_L (m/s)	H _{cc}	D_{aq} (m ² /s)
Nitrogen, N ₂	-	65	1.9×10 ⁻⁹
Oxygen, O ₂	2.0×10^{-5}	30	2.1×10 ⁻⁹
Ethanol, C ₂ H ₅ OH	4.1×10 ⁻⁷	2.7×10 ⁻⁴	1.2×10 ⁻⁹

1) Determine which phase controls the mass transfer for each compound. Assume k_G/k_L of 100. Show your reasoning.

Solution)

For N₂: $\frac{R_L}{R_G} = \frac{k_G H_{cc}}{k_L} = 100 \times 65 \gg 1$

liquid phase controls

For O_2 : $\frac{R_L}{R_G} = \frac{k_G H_{cc}}{k_L} = 100 \times 30 = 3000 \gg 1$

liquid phase controls

For
$$C_2 H_5 OH$$
:
 $\frac{R_L}{R_G} = \frac{k_G H_{cc}}{k_L} = 100 \times (2.7 \times 10^{-4}) = 0.027 \ll 1$ gas phase controls

Film theory

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2) Assuming that film theory is applicable, predict the K_L for nitrogen.

Solution)

If film theory is valid, then

$$k_L \propto D_L$$
$$\frac{k_{L,N_2}}{k_{L,O_2}} = \frac{D_{L,N_2}}{D_{L,O_2}}$$

For both $N_2 \& O_2$, liquid phase controls the mass transfer. Therefore: $K_L \approx k_L$

We conclude:

$$K_{L,N_2} = k_{L,N_2} = k_{L,O_2} \times \frac{D_{L,N_2}}{D_{L,O_2}}$$
$$= (2.0 \times 10^{-5} \text{ m/s}) \times \frac{1.9 \times 10^{-9} \text{ m}^2/\text{s}}{2.1 \times 10^{-9} \text{ m}^2/\text{s}} = 1.8 \times 10^{-5} \text{ m/s}$$

Predicting conc. change in water

Q: You bought a bottle of "super oxygen water" from a market, which is highly supersaturated with oxygen (dissolved oxygen concentration (DO) = 60 mg/L). You poured 200 cm³ of the drink to a cup in a cylindrical shape with an inner diameter of 8 cm and left it for 3 hours. What will be the DO of the drink then? Use an overall mass transfer coefficient (K_L) of 1.00×10⁻² m/h and the saturation DO of 8.3 mg/L.

Solution)

$$a = \frac{A}{V} = \frac{\pi d^2}{V} = \frac{\pi \cdot (8 \ cm)^2}{200 \ cm^3} = 0.251 \ cm^{-1}$$

 $K_L a = (1.00 \times 10^{-2} \ m/h) \times (100 \ cm/m) \times (0.251 \ cm^{-1}) = 0.251 \ h^{-1}$

$$\frac{dC_{bulk}^{L}}{dt} = -K_L a \left(C_{bulk}^{L} - C_{bulk}^{L*} \right)$$

$$\frac{dC_{bulk}^{L}}{\left(C_{bulk}^{L}-C_{bulk}^{L*}\right)}=-K_{L}a\cdot dt$$

$$\int_{C_{bulk}^{L}(t=0)}^{C_{bulk}^{L}(t=t)} \frac{dC_{bulk}^{L}}{\left(C_{bulk}^{L} - C_{bulk}^{L*}\right)} = -K_{L}a \cdot \int_{0}^{t} dt$$

$$ln\{C_{bulk}{}^{L} - C_{bulk}{}^{L*}\}\Big|_{C_{bulk}{}^{L}(t=0)}^{C_{bulk}{}^{L}(t=t)} = -K_{L}a \cdot t\Big|_{0}^{t}$$

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$$ln \frac{\{C_{bulk}^{L} (t=t)\} - C_{bulk}^{L*}}{\{C_{bulk}^{L} (t=0)\} - C_{bulk}^{L*}} = -K_{L}a \cdot t$$

$$\{C_{bulk}{}^{L} (t = t)\} = \{C_{bulk}{}^{L} (t = 0)\} \cdot e^{-K_{L}a \cdot t} + C_{bulk}{}^{L*} \cdot (1 - e^{-K_{L}a \cdot t})$$
$$= 60 \ mg/L \cdot e^{-0.251 \ h^{-1} \cdot 3 \ h} + 8.3 \ mg/L \cdot (1 - e^{-0.251 \ h^{-1} \cdot 3 \ h})$$

= 32.6 mg/L