Interphase mass transfer III:
Applications

## Flux to concentration change (in water)

$$
\begin{aligned}
& J_{t o t}=-K_{L}\left(C_{b u l k}{ }^{L}-C_{\text {bulk }}{ }^{L *}\right) \quad \text { Flux rate per unit area } \\
& A \cdot J_{\text {tot }}=-K_{L} \cdot A\left(C_{b u l k}^{L}-C_{b u l k}{ }^{L *}\right) \quad \text { Total flux (A is area of air-water interface) } \\
& \frac{\boldsymbol{d} \boldsymbol{C}_{\text {bulk }}{ }^{L}}{\boldsymbol{d t}}=\left(\frac{A}{V}\right) J_{t o t}=-K_{L}\left(\frac{A}{V}\right)\left(C_{b_{b u l k}}{ }^{L}-C_{b u l k}{ }^{L *}\right)=-\boldsymbol{K}_{L} \boldsymbol{a}\left(\boldsymbol{C}_{\text {bulk }}{ }^{L}-\boldsymbol{C}_{\text {bulk }}{ }^{L^{*}}\right)
\end{aligned}
$$

This is the rate of change in concentration in water

$$
\begin{aligned}
& a=\text { interfacial area for mass transfer per unit volume, } A / V\left[L^{-1}\right] \\
& V=\text { volume in which concentration is changing }\left[L^{3}\right] \\
& \boldsymbol{K}_{L} a=\text { volumetric mass transfer coefficient }\left[T^{-1}\right]
\end{aligned}
$$

## Mass transfer example: change in stream DO

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

$$
\begin{array}{ll}
K_{L}=\left(\frac{D_{L} u}{H}\right)^{0.5}=k_{L} \\
K_{L} a=\frac{\left(D_{L} u\right)^{0.5}}{H^{1.5}} & \begin{array}{l}
u=\text { stream velocity, } m / s \\
H=1 / a=\text { average stream depth, } m \\
D_{L}=\text { liquid phase diffusivity, } m^{2} / \mathrm{s}
\end{array}
\end{array}
$$

## Mass transfer example: change in stream DO

- Applying surface renewal model:

O'Connor and Dobbins hypothesized that

$$
s_{L}=\frac{\text { Avg.vertical velocity by turbulence }}{\text { Avg. mixing length }}=\frac{0.1 u}{0.1 \mathrm{H}}=\frac{u}{H}
$$

Therefore,

$$
K_{L} \approx k_{L}=\left(D_{L} s_{L}\right)^{1 / 2}=\left(\frac{D_{L} u}{H}\right)^{1 / 2}
$$

## Mass transfer example: change in stream DO

- Applying boundary layer theory:

$$
\begin{aligned}
& k_{L}=\frac{(S h)_{L} D_{L}}{d}=\frac{a_{2}(R e)^{a_{3}}(v)^{a_{4}} D_{L}^{1-a_{4}}}{d}=a_{2} d^{\left(a_{3}-1\right)} u^{a_{3}} v^{\left(a_{4}-a_{3}\right)} D_{L}^{\left(1-a_{4}\right)} \\
& \text { If } a_{2}=1.0 ; a_{3} \& a_{4}=0.5: \\
& \quad K_{L} \approx k_{L}=\left(\frac{D_{L} u}{d}\right)^{0.5}
\end{aligned}
$$

## Boundary layer theory: applications

Transfer to particle surface in stagnant fluid:

$$
\frac{k_{L} d}{D_{L}}(S h)_{L}=a_{1}+a_{2}(R e)^{a_{3}}(S c)_{L}^{a}
$$

$$
\begin{array}{|}
\text { Re= } \frac{d \times u}{v}=\frac{d \times u \times \rho}{\mu} \\
(S c)_{L}{ }^{a_{4}}=\frac{v}{D_{L}}=\frac{\mu}{D_{L} \rho}
\end{array}
$$

Here, $a_{1}=2$

$$
\begin{aligned}
& k_{L}=\frac{2 D_{L}}{d_{p}}=\frac{D_{L}}{r_{p}} \approx \frac{1 \times 10^{-9}}{r_{p}} \mathrm{~m} / \mathrm{sec} \\
& a=\frac{\text { area }}{\text { volume }}=\frac{6}{d_{p}} \mathrm{~m}^{-1}
\end{aligned}
$$

If resistance is dominant at liquid phase,

$$
K_{L} a \approx k_{L} a \approx \frac{10^{-8}}{d_{p}^{2}} \sec ^{-1}
$$

## 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 | $\boldsymbol{K}_{\boldsymbol{L}}(\mathbf{m} / \mathbf{s})$ | $\boldsymbol{H}_{\boldsymbol{c} \boldsymbol{c}}$ | $\boldsymbol{D}_{a q}\left(\mathbf{m}^{2} / \mathbf{s}\right)$ |
| :---: | :---: | :---: | :---: |
| Nitrogen, $\mathrm{N}_{2}$ | - | 65 | $1.9 \times 10^{-9}$ |
| Oxygen, $\mathrm{O}_{2}$ | $2.0 \times 10^{-5}$ | 30 | $2.1 \times 10^{-9}$ |
| Ethanol, $\mathrm{C}_{2} \mathrm{H}_{5} \mathrm{OH}$ | $4.1 \times 10^{-7}$ | $2.7 \times 10^{-4}$ | $1.2 \times 10^{-9}$ |

1) Determine which phase controls the mass transfer for each compound. Assume $k_{G} / k_{L}$ of 100 . Show your reasoning.

## Solution)

For $N_{2}$ :

$$
\frac{R_{L}}{R_{G}}=\frac{k_{G} H_{c c}}{k_{L}}=100 \times 65 \gg 1
$$

liquid phase controls

For $\mathrm{O}_{2}$ :

$$
\frac{R_{L}}{R_{G}}=\frac{k_{G} H_{c c}}{k_{L}}=100 \times 30=3000 \gg 1
$$

liquid phase controls

For $\mathrm{C}_{2} \mathrm{H}_{5} \mathrm{OH}$ :

$$
\frac{R_{L}}{R_{G}}=\frac{k_{G} H_{c c}}{k_{L}}=100 \times\left(2.7 \times 10^{-4}\right)=0.027 \ll 1 \quad \text { gas phase controls }
$$

## Film theory

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:

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2) Assuming that film theory is applicable, predict the $K_{L}$ for nitrogen.

## Solution)

If film theory is valid, then

$$
\begin{aligned}
& k_{L} \propto D_{L} \\
& \frac{k_{L, N_{2}}}{k_{L, O_{2}}}=\frac{D_{L, N_{2}}}{D_{L, O_{2}}}
\end{aligned}
$$

For both $\mathrm{N}_{2} \& \mathrm{O}_{2}$, liquid phase controls the mass transfer. Therefore:

$$
K_{L} \approx k_{L}
$$

We conclude:

$$
\begin{aligned}
K_{L, N_{2}} & =k_{L, N_{2}}=k_{L, O_{2}} \times \frac{D_{L, N_{2}}}{D_{L, O_{2}}} \\
& =\left(2.0 \times 10^{-5} \mathrm{~m} / \mathrm{s}\right) \times \frac{1.9 \times 10^{-9} \mathrm{~m}^{2} / \mathrm{s}}{2.1 \times 10^{-9} \mathrm{~m}^{2} / \mathrm{s}}=\mathbf{1 . 8} \times \mathbf{1 0}^{-\mathbf{5}} \mathrm{m} / \mathrm{s}
\end{aligned}
$$

## 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) $=60 \mathrm{mg} / \mathrm{L}$ ). You poured $200 \mathrm{~cm}^{3}$ 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 $\left(K_{L}\right)$ of $1.00 \times 10^{-2} \mathrm{~m} / \mathrm{h}$ and the saturation DO of $8.3 \mathrm{mg} / \mathrm{L}$.

## Solution)

$$
\begin{aligned}
& a=\frac{A}{V}=\frac{\pi d^{2}}{V}=\frac{\pi \cdot(8 \mathrm{~cm})^{2}}{200 \mathrm{~cm}^{3}}=0.251 \mathrm{~cm}^{-1} \\
& K_{L} a=\left(1.00 \times 10^{-2} \mathrm{~m} / \mathrm{h}\right) \times(100 \mathrm{~cm} / \mathrm{m}) \times\left(0.251 \mathrm{~cm}^{-1}\right)=0.251 \mathrm{~h}^{-1} \\
& \frac{d C_{b u l k}{ }^{L}}{d t}=-K_{L} a\left(C_{b u l k}{ }^{L}-C_{b u l k}{ }^{L *}\right) \\
& \frac{d C_{b u l k}^{L}}{\left(C_{b u l k}{ }^{L}-C_{b u l k}{ }^{L *}\right)}=-K_{L} a \cdot d t \\
& \int_{C_{b u l k}{ }^{L}(t=0)}^{C_{b u l k}{ }^{L}(t=t)} \frac{d C_{b u l k}{ }^{L}}{\left(C_{b u l k}^{L}-C_{b u l k}^{L *}\right)}=-K_{L} a \cdot \int_{0}^{t} d t \\
& \left.\ln \left\{C_{b u l k}{ }^{L}-C_{b u l k}{ }^{L *}\right\}\right|_{C_{b u l k}{ }^{L}(t=0)} ^{C_{b u l k}^{L}(t=t)}=-\left.K_{L} a \cdot t\right|_{0} ^{t}
\end{aligned}
$$

$$
\begin{aligned}
& \ln \frac{\left\{C_{\text {bulk }}{ }^{L}(t=t)\right\}-C_{\text {bulk }}{ }^{L *}}{\left\{C_{\text {bulk }}{ }^{L}(t=0)\right\}-C_{\text {bulk }}{ }^{L *}}=-K_{L} a \cdot t \\
& \left\{C_{b u l k}{ }^{L}(t=t)\right\}=\left\{C_{\text {bulk }}{ }^{L}(t=0)\right\} \cdot e^{-K_{L} a \cdot t}+C_{b u l k}{ }^{L *} \cdot\left(1-e^{-K_{L} a \cdot t}\right) \\
& =60 \mathrm{mg} / \mathrm{L} \cdot e^{-0.251 h^{-1} .3 h}+8.3 \mathrm{mg} / \mathrm{L} \cdot\left(1-e^{-0.251 h^{-1} .3 h}\right) \\
& =32.6 \mathrm{mg} / \mathrm{L}
\end{aligned}
$$

