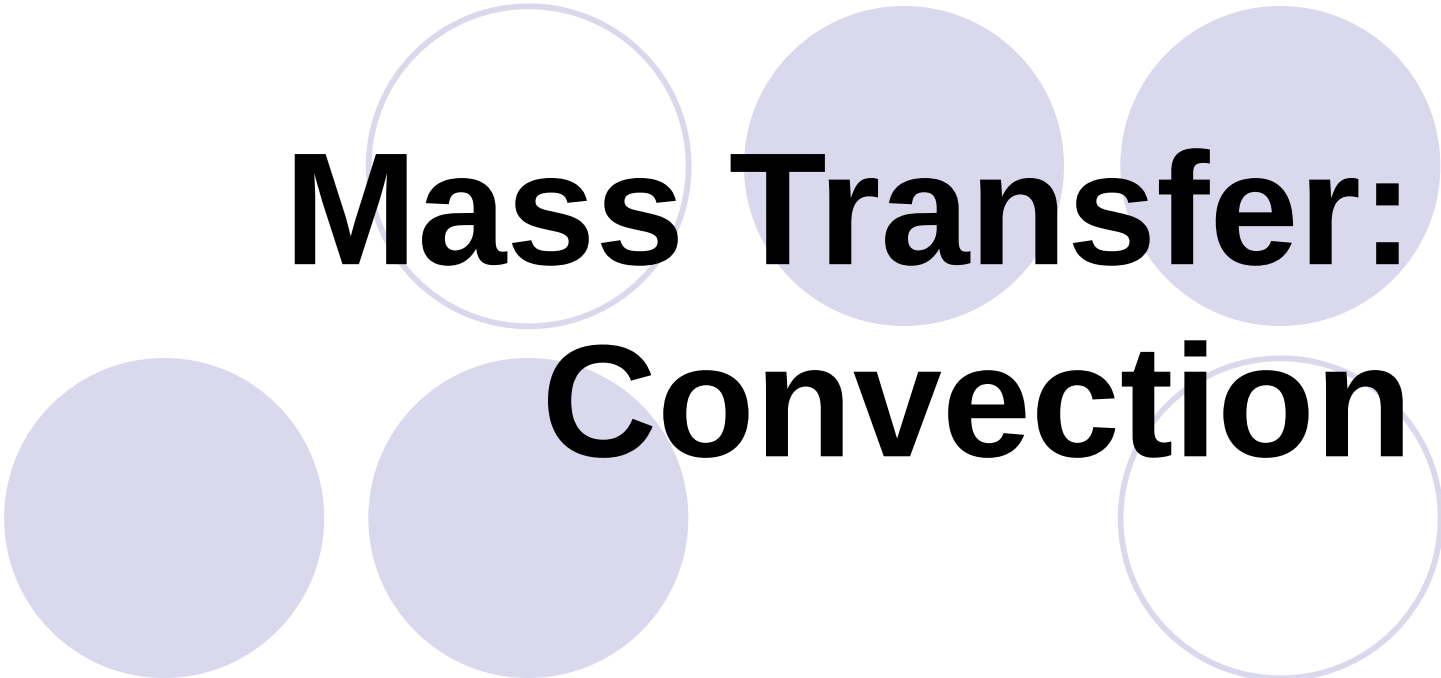






Mass Transfer: Convection

Relationships between concentrations in a binary system.

	mass fraction ω [-]	mole fraction x [-]	absolute humidity $H \left[\frac{\text{kg} - \text{A}}{\text{kg} - \text{B}} \right]$	mole ratio $X \left[\frac{\text{mol} - \text{A}}{\text{mol} - \text{B}} \right]$
mass fraction ω [-]	ω	$\frac{x}{\frac{M_B}{M_A} + \left\{ 1 - \frac{M_B}{M_A} \right\} x}$	$\frac{H}{1 + H}$	$\frac{X}{\frac{M_B}{M_A} + X}$
mole fraction x [-]	$\frac{\omega}{\frac{M_A}{M_B} + \left\{ 1 - \frac{M_A}{M_B} \right\} \omega}$	x	$\frac{H}{\frac{M_A}{M_B} + H}$	$\frac{X}{1 + X}$
absolute humidity $H \left[\frac{\text{kg} - \text{A}}{\text{kg} - \text{B}} \right]$	$\frac{\omega}{1 - \omega}$	$\left(\frac{x}{1 - x} \right) \left(\frac{M_A}{M_B} \right)$	H	$\left(\frac{M_A}{M_B} \right) X$
mole ratio $X \left[\frac{\text{mol} - \text{A}}{\text{mol} - \text{B}} \right]$	$\left(\frac{M_B}{M_A} \right) \left(\frac{\omega}{1 - \omega} \right)$	$\left(\frac{x}{1 - x} \right)$	$\left(\frac{M_B}{M_A} \right) H$	X

Relationships between various definitions of concentration in a multicomponent system.

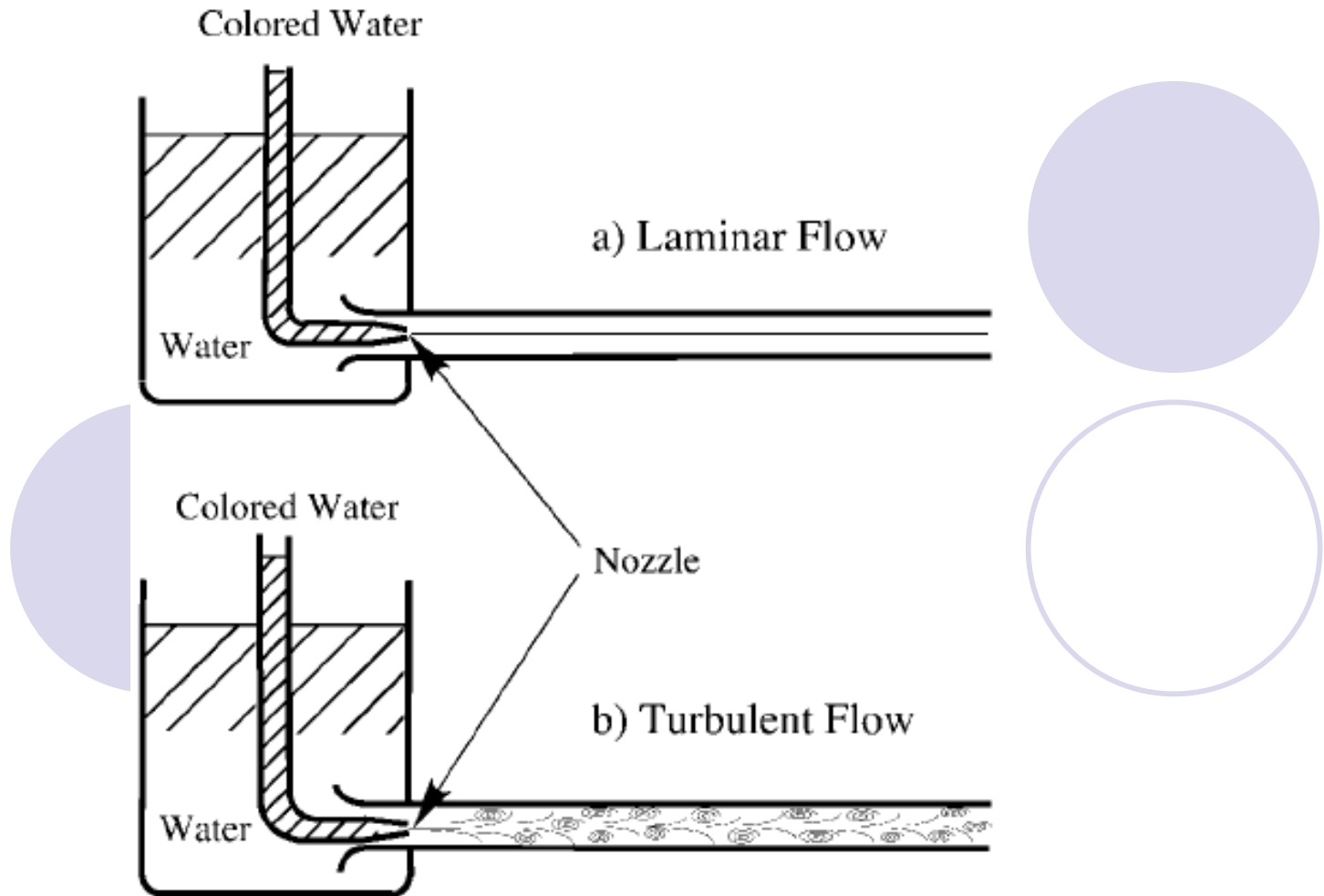
	mass fraction ω_A [-]	mole fraction x_A [-]	partial density ρ_A [kg m ⁻³]	molar density c_A [kmol m ⁻³]	partial pressure p_A [kPa]
mass fraction ω_A [-]	ω	$\frac{x_A M_A}{\sum_i x_i M_i}$	$\frac{\rho_A}{\sum_i \rho_i}$	$\frac{c_A M_A}{\sum_i c_i M_i}$	$\frac{p_A M_A}{\sum_i p_i M_i}$
mole fraction x_A [-]	$\frac{(\omega_A/M_A)}{\sum_i (\omega_i/M_i)}$	x_A	$\frac{\rho_A/M_A}{\sum_i (\rho_i/M_i)}$	$\frac{c_A}{\sum_i c_i}$	$\frac{p_A}{\sum_i p_i}$
partial density ρ_A [kg m ⁻³]	$\rho \omega_A$	$\frac{\rho x_A M_A}{\sum_i x_i M_i}$	ρ_A	$c_A M_A$	$\frac{M_A p_A}{RT}$
molar density c_A [kmol m ⁻³]	$\frac{\rho \omega_A}{M_A}$	$c x_A$	$\frac{\rho_A}{M_A}$	c_A	$\frac{p_A}{RT}$
partial pressure p_A [kPa]	$\frac{(\omega_A/M_A)P}{\sum_i (\omega_i/M_i)}$	$P x_A$	$\frac{RT \rho_A}{M_A}$	$c_A RT$	p_A
Mixture: $\sum_i x_i = 1$, $\sum_i \omega_i = 1$, $\rho = \sum_i \rho_i$, $c = \sum_i c_i$, $P = \sum_i p_i$ $M = \sum_i M_i x_i = \left(\sum_i \frac{\omega_i}{M_i} \right)^{-1}$					

Mass transfer coefficients.

Mass transfer coefficient	Unit	Definition	Driving force	Phase
k_y	$[\text{kmol m}^{-2} \text{ s}^{-1}]$	$N_A^* = k_y (\gamma_s - \gamma_\infty)$	$\Delta \gamma$	Gas phase
k_G	$[\text{kmol m}^{-2} \text{ s}^{-1} \text{ kPa}^{-1}]$	$N_A^* = k_G (p_s - p_\infty)$	Δp	
k_Y	$[\text{kmol m}^{-2} \text{ s}^{-1}]$	$N_A^* = k_Y (Y_s - Y_\infty)$	ΔY	
k	$[\text{m s}^{-1}]$	$N_A = \rho_G k (\omega_{Gs} - \omega_{G\infty})$	$\Delta \omega_G$	
k_H	$[\text{kg m}^{-2} \text{ s}^{-1}]$	$N_A = k_H (H_s - H_\infty)$	ΔH	
k_L	$[\text{m s}^{-1}]$	$N_A^* = k_L (c_s - c_\infty)$	Δc	Liquid phase
k_x	$[\text{kmol m}^{-2} \text{ s}^{-1}]$	$N_A^* = k_x (x_s - x_\infty)$	Δx	
k_X	$[\text{kmol m}^{-2} \text{ s}^{-1}]$	$N_A^* = k_X (X_s - X_\infty)$	ΔX	
k	$[\text{m s}^{-1}]$	$N_A = \rho_L k (\omega_{Ls} - \omega_{L\infty})$	$\Delta \omega_L$	
c = molar density $[\text{mol m}^{-3}]$, H = absolute humidity $[-]$, M_A = molecular weight $[\text{kg kmol}^{-1}]$, N_A = mass flux $[\text{kg m}^{-2} \text{ s}^{-1}]$, $N_A^* = N_A/M_A$ = molar flux $[\text{kmol m}^{-2} \text{ s}^{-1}]$, p = partial pressure $[\text{kPa}]$, x, γ = mole fraction $[-]$, $X = x/(1 - x)$ $[-]$, $Y = \gamma/(1 - x)$ $[-]$, ω = mass fraction $[-]$.				

Governing Equations of Mass Transfer

Laminar and Turbulent Flow

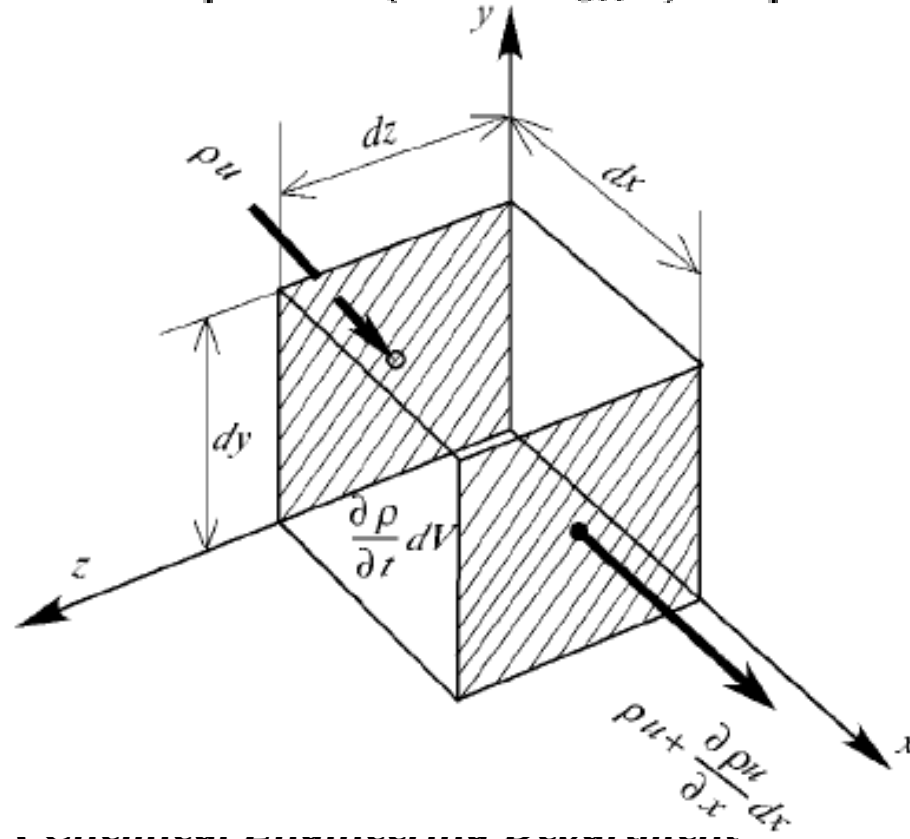


Continuity Equation and Diffusion Equation

(Rate of accumulation of mass in dV) =

(Rate of mass flowing into dV) – (Rate of mass flowing out from dV)

$$\left\{ \rho u \Big|_x - \rho u \Big|_{x+dx} \right\} dydz = \left\{ \rho u - \left(\rho u + \frac{\partial \rho u}{\partial x} dx \right) \right\} dydz = - \left(\frac{\partial \rho u}{\partial x} \right) dV$$



Continuity Equation

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0$$

Diffusion Equation in Terms of Mass Fraction

The conservation of mass for component **A** in a small volume element of a fluid mixture gives the following equation, *the continuity equation for component A*:

$$\frac{\partial \rho_A}{\partial t} + \frac{\partial \rho_A u_A}{\partial x} + \frac{\partial \rho_A v_A}{\partial y} + \frac{\partial \rho_A w_A}{\partial z} - r_A M_A = 0$$

The components of the velocity of **A** are related to the components of the local mass average velocity through the definition of mass diffusional flux:

$$J_{Ax} \equiv \rho_A (u_A - u)$$

$$J_{Ay} \equiv \rho_A (v_A - v)$$

$$J_{Az} \equiv \rho_A (w_A - w)$$

the following equation for the mass fraction:

$$\rho_A = \rho \omega_A$$

we have the following equations:

$$\frac{\partial \rho_A}{\partial t} = \frac{\partial \rho \omega_A}{\partial t} = \rho \frac{\partial \omega_A}{\partial t} + \omega_A \frac{\partial \rho}{\partial t}$$

$$\frac{\partial \rho_A u_A}{\partial x} = \frac{\partial \rho u \omega_A}{\partial x} + \frac{\partial}{\partial x} \rho \omega_A (u_A - u) = \rho u \frac{\partial \omega_A}{\partial x} + \omega_A \frac{\partial \rho u}{\partial x} + \frac{\partial J_{Ax}}{\partial x}$$

$$\frac{\partial \rho_A v_A}{\partial y} = \rho v \frac{\partial \omega_A}{\partial y} + \omega_A \frac{\partial \rho v}{\partial y} + \frac{\partial J_{Ay}}{\partial y}$$

$$\frac{\partial \rho_A w_A}{\partial z} = \rho w \frac{\partial \omega_A}{\partial z} + \omega_A \frac{\partial \rho w}{\partial z} + \frac{\partial J_{Aw}}{\partial z}$$

Substituting these equations

$$\rho \frac{\partial \omega_A}{\partial t} + \rho u \frac{\partial \omega_A}{\partial x} + \rho v \frac{\partial \omega_A}{\partial y} + \rho w \frac{\partial \omega_A}{\partial z} + \left(\frac{\partial J_{Ax}}{\partial x} + \frac{\partial J_{Ay}}{\partial y} + \frac{\partial J_{Az}}{\partial z} \right) - r_A M_A = 0$$

apply *Fick's law* of diffusion:

$$J_{Ax} = -\rho D \frac{\partial \omega_A}{\partial x}$$

$$J_{Ay} = -\rho D \frac{\partial \omega_A}{\partial y}$$

$$J_{Az} = -\rho D \frac{\partial \omega_A}{\partial z}$$

we obtain the following equation:

$$\frac{\partial \omega_A}{\partial t} + u \frac{\partial \omega_A}{\partial x} + v \frac{\partial \omega_A}{\partial y} + w \frac{\partial \omega_A}{\partial z} = D \left(\frac{\partial^2 \omega_A}{\partial x^2} + \frac{\partial^2 \omega_A}{\partial y^2} + \frac{\partial^2 \omega_A}{\partial z^2} \right)$$

Diffusion Equation in Terms of Mole Fraction

for the case without chemical reaction ($r_A = 0$) by use of the following equation for the partial density:

$$\rho_A = c_A M_A = c x_A M_A$$

we have the following equation:

$$\left(\frac{\partial x_A}{\partial t} + u_A^* \frac{\partial x_A}{\partial x} + v_A^* \frac{\partial x_A}{\partial y} + w_A^* \frac{\partial x_A}{\partial z} \right) + \frac{1}{c} \left(\frac{\partial J_{Ax}^*}{\partial x} + \frac{\partial J_{Ay}^*}{\partial y} + \frac{\partial J_{Az}^*}{\partial z} \right) = 0$$

$$J_{Ax}^* = c x_A (u_A - u^*)$$

$$J_{Ay}^* = c x_A (v_A - v^*)$$

$$J_{Az}^* = c x_A (w_A - w^*)$$

If we further assume a binary system of constant physical properties, then the well-known *Fick's law of diffusion* also applies:

$$J_{Ax}^* = -cD \frac{\partial x_A}{\partial x}$$

$$J_{Ay}^* = -cD \frac{\partial x_A}{\partial y}$$

$$J_{Az}^* = -cD \frac{\partial x_A}{\partial z}$$

Substituting the above equations, we obtain the following equation:

$$\begin{aligned} & \left\{ \frac{\partial x_A}{\partial t} + u \frac{\partial x_A}{\partial x} + v \frac{\partial x_A}{\partial y} + w \frac{\partial x_A}{\partial z} - D \left(\frac{\partial^2 x_A}{\partial x^2} + \frac{\partial^2 x_A}{\partial y^2} + \frac{\partial^2 x_A}{\partial z^2} \right) \right\} \\ & + \left\{ (u^* - u) \frac{\partial x_A}{\partial x} + (v^* - v) \frac{\partial x_A}{\partial y} + (w^* - w) \frac{\partial x_A}{\partial z} \right\} = 0 \end{aligned}$$

The component of the velocity difference in the x-coordinate can be expressed by

$$(u^* - u) = (x_A u_A + x_B u_B) - (\omega_A u_A + \omega_B u_B) = \frac{x_A x_B (M_B - M_A)}{\bar{M}} (u_A - u_B)$$

Similar relationships are obtained for the components in the y- and z-coordinates.

if either of the following conditions is satisfied:

Case 1) Equal molecular weights of the two components, $M_A = M_B$

Case 2) The concentration of one of the two components is very low,

$$x_A \approx 0 \quad \text{or} \quad x_B = 1 - x_A \approx 0$$

Under these special conditions, * can be approximated by the following equation, and a familiar diffusion equation in terms of mole fractions is obtained.

$$\frac{\partial x_A}{\partial t} + u \frac{\partial x_A}{\partial x} + v \frac{\partial x_A}{\partial y} + w \frac{\partial x_A}{\partial z} = D \left(\frac{\partial^2 x_A}{\partial x^2} + \frac{\partial^2 x_A}{\partial y^2} + \frac{\partial^2 x_A}{\partial z^2} \right)$$

The Equation of Motion (Navier–Stokes Equation)

The equation of motion for a fluid of constant physical properties in Cartesian coordinates can be written as follows:

$$\begin{aligned}\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} &= -\frac{1}{\rho} \frac{\partial P}{\partial x} + \frac{\mu}{\rho} \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) + g_x \\ \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} &= -\frac{1}{\rho} \frac{\partial P}{\partial y} + \frac{\mu}{\rho} \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} \right) + g_y \\ \frac{\partial w}{\partial t} + u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} &= -\frac{1}{\rho} \frac{\partial P}{\partial z} + \frac{\mu}{\rho} \left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right) + g_z\end{aligned}$$

The Energy Equation

The energy equation is also derived by application of *the law of conservation of energy*. Here, we present the energy equation for a fluid of constant physical properties under moderate flow conditions, where the effect of viscous dissipation is negligibly small.

$$\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} + w \frac{\partial T}{\partial z} = \frac{\kappa}{\rho c_p} \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right)$$

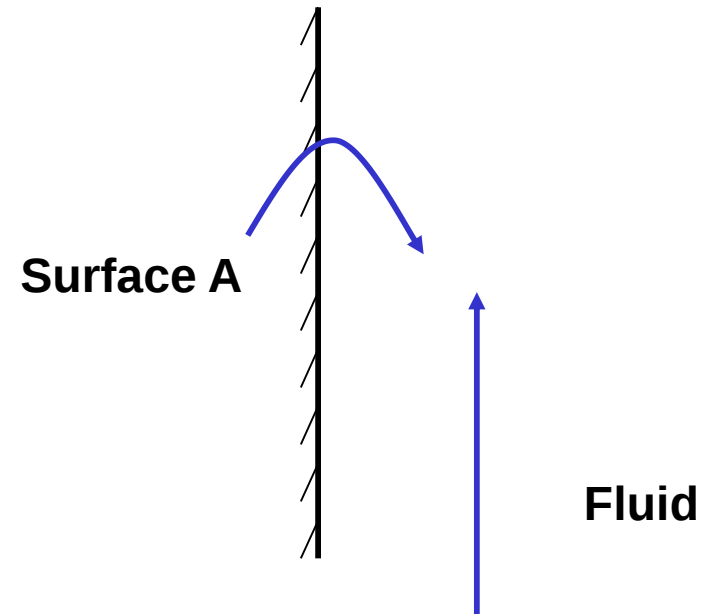
Examples of Convective Mass Transfer

- ➡ Two fluids, immiscible with each other, flowing parallel or counter-current with each other and containing solutes soluble to both.
- ➡ Fluid flowing against a solid surface. The solute is leached out from the solid surface by the flowing fluid.

Mechanism of Turbulent Transfer

➡ Laminar flow

fluid flows in streamlines and its behavior can be described mathematically



➡ Turbulent flow

the fluid is moving in rapid, random motion as chunks or large eddies

Three Regions of Mass Transfer

- Viscous sublayer
- Buffer region
- Turbulent region

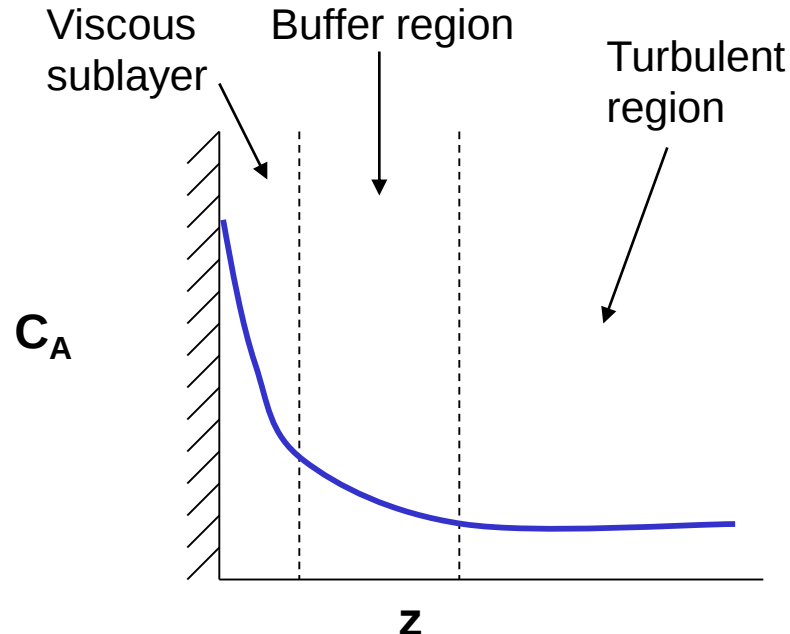
Controlling Mechanism

Diffusion

Diffusion and Convection

Convection

Typical
concentration
profile



Mass Transfer Coefficients

For turbulent mass transfer:

$$_V J_A = -(D_{AB} + \varepsilon_M) \frac{dC_A}{dz}$$

$$_M J_A = -C(D_{AB} + \varepsilon_M) \frac{dx_A}{dz}$$

where : ε_M = eddy mass diffusivity

Mass Transfer Coefficients

► For equimolar counter-diffusion

$$N_A = \frac{(D_{AB} + \varepsilon_M)}{\Delta z} (C_{A1} - C_{A2})$$

$$N_A = k'_c (C_{A1} - C_{A2})$$

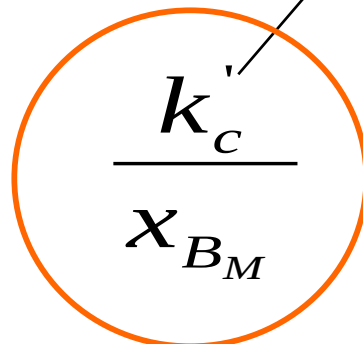
Mass transfer
coefficient

Mass Transfer Coefficients

► For unimolar diffusion

$$N_A = \frac{(D_{AB} + \varepsilon_M)}{\Delta z} \frac{(C_{A1} - C_{A2})}{x_{B_M}}$$

$$N_A = k_c (C_{A1} - C_{A2})$$


$$\frac{k'_c}{x_{B_M}}$$

Summary

Equimolar counter-diffusion

Gases
$$N_A = k'_c(C_{A1} - C_{A2}) = k'_G(P_{A1} - P_{A2}) = k'_y(y_{A1} - y_{A2})$$

Liquids
$$N_A = k'_c(C_{A1} - C_{A2}) = k'_L(C_{A1} - C_{A2}) = k'_x(x_{A1} - x_{A2})$$

Unimolar diffusion

Gases
$$N_A = k_c(C_{A1} - C_{A2}) = k_G(P_{A1} - P_{A2}) = k_y(y_{A1} - y_{A2})$$

Liquids
$$N_A = k_c(C_{A1} - C_{A2}) = k_L(C_{A1} - C_{A2}) = k_x(x_{A1} - x_{A2})$$

Conversions

Gases

$$\begin{aligned} k'_c C &= k'_c \frac{P}{RT} = k_c \frac{P_{B_M}}{RT} = k'_G P = k_G P_{B_M} \\ &= k_y y_{B_M} = k'_y = k_c y_{B_M} C = k_G y_{B_M} P \end{aligned}$$

Liquids

$$k'_c = k'_L C = k_L x_{B_M} C = k'_L \frac{\rho}{M} = k'_x = k_x x_{B_M}$$

Units

Units

$$k'_c, k_c, k_L, k'_L \quad \frac{m}{s}, \quad \frac{ft}{h}$$

$$k'_x, k_x, k_y, k'_y \quad \frac{kgmol}{s - m^2 - mol \text{ frac}}, \quad \frac{lbmol}{h - ft^2 - mol \text{ frac}}$$

$$k'_G, k_G \quad \frac{kgmol}{s - m^2 - Pa}, \quad \frac{lbmol}{h - ft^2 - atm}$$

Estimation of Mass Transfer Coefficients

Dimensionless Numbers Used to Correlate Data

- ➡ **Schmidt No. (Sc)** – analogous to P_r ; ratio of the shear component of diffusivity to the diffusivity to mass transfer; physically relates the thickness of the hydrodynamic boundary layer and mass-transfer boundary layer

$$Sc = \frac{\mu}{\rho D_{AB}}$$

Dimensionless numbers for heat and mass transfer

- Analogies among heat and mass transfer

Heat	Mass
Nu	Sh
Pr	Sc
Gr	Gr_x
$Pe = Re \cdot Pr$	$Pe = Re \cdot Sc$
j_H	j_D

Estimation of Mass Transfer Coefficients

Dimensionless Numbers Used to Correlate Data

➡ Sherwood No. (Sh)

$$Sh = k'_c \frac{L}{D_{AB}} = k_c y_{B_M} \frac{L}{D_{AB}} = \frac{k'_x}{c} \frac{L}{D_{AB}} \dots\dots$$

➡ Stanton No. (St)

$$St = \frac{k'_c}{\nu} = \frac{k'_y}{G_M} = \frac{k'_G P}{G_M} \dots\dots$$

where

$$G_M = \frac{\nu \rho}{M_{ave}} = \nu C$$

Estimation of Mass Transfer Coefficients

Dimensionless Numbers Used to Correlate Data

► J_D Factor

$$J_D = \frac{k'_c}{\nu} (Sc)^{2/3} = k'_G \frac{P}{G_M} (Sc)^{2/3} = \dots\dots\dots \frac{Sh}{(Re Sc^{1/3})}$$

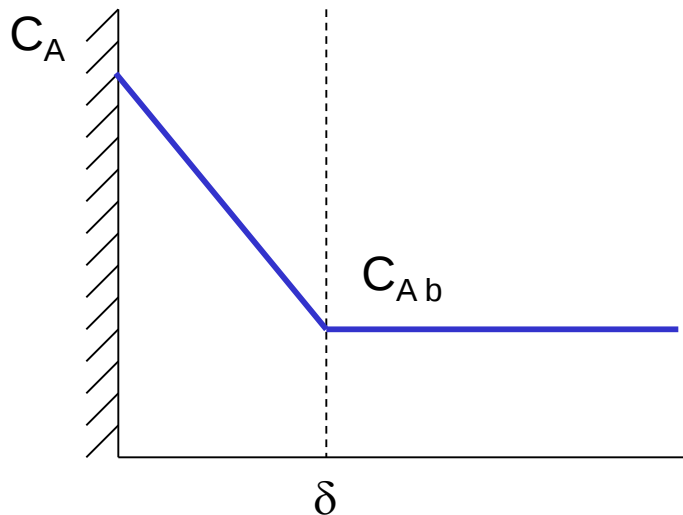
For heat transfer

$$J_H = \frac{h}{c_p G} (Pr)^{2/3}$$

Theoretical Mass Transfer Models

► Film theory

The resistance to mass transfer in a given turbulent phase is confined in a thin, stagnant region at the interface (film)



Consequence: The entire concentration difference ($C_A - C_{ab}$) is attributed to molecular diffusion within an effective film thickness δ

Theoretical Mass Transfer Models

► Penetration theory

Higbie states that in many situations the time exposure of a fluid to mass transfer is short, so that the concentration gradient of the film theory would not have time to develop

$$k_L = \left(\frac{D_{AB}}{\pi\theta} \right)^{1/2}$$

In the absorption of gases from bubbles or absorption by wetted-wall columns, the mass transfer surface is formed instantaneously and transient diffusion of the material takes place. Under these circumstances, we can neglect the convective terms in the diffusion equation and so it reduces to a similar equation as applies in the case of transient heat conduction:

$$\frac{\partial \omega}{\partial t} = D \frac{\partial^2 \omega}{\partial x^2}$$

The boundary conditions are:

$$t = 0, \quad x > 0 : \quad \omega = \omega_{\infty}$$

$$t > 0, \quad x = 0 : \quad \omega = \omega_s$$

the solution for the above boundary conditions is given by the following equation

$$\frac{\omega_s - \omega}{\omega_s - \omega_{\infty}} = \operatorname{erf} \left(\frac{x}{2\sqrt{Dt}} \right) \quad \operatorname{erf} (x) \equiv \frac{2}{\sqrt{\pi}} \int_0^x \exp(-z^2) dz$$

$$N_A(t) = \rho \sqrt{\frac{D}{\pi t}} (\omega_s - \omega_\infty)$$

The mass transfer coefficient is given by:

$$k(t) = \sqrt{\frac{D}{\pi t}}$$

The average mass transfer coefficient during a time interval t_c [s] is obtained by integrating

$$\bar{k} = \frac{1}{t_c} \int_0^{t_c} k(t) dt = 2 \sqrt{\frac{D}{\pi t_c}}$$

Theoretical Mass Transfer Models

► Surface-Renewal theory

Danckwerts pointed out that the Higbie theory with its contact-time exposure of the eddies of the fluid at the surface is a special case of what may be a more realistic picture, where the eddies are exposed for varying lengths of time. The liquid-gas interface is then a mosaic of surface elements of different exposure-time histories.

$$k_{L_{ave}} = \sqrt{D_{AB} S}$$

S = fractional rate of replacement of elements

Example

A 3 mm diameter air bubble is introduced into water from the bottom of a container of depth 0.5 m. Calculate the amount of oxygen absorbed by the single bubble, if it rises at a velocity of 2 m s⁻¹, the pressure inside the bubble is 1 atmosphere (101.325 kPa), and the water temperature is 20 C. Henry's constant of oxygen in water and the diffusion coefficient of oxygen in water at 20 C are given as follows:

$$H = 4052 \text{ MPa}, D_L = 2.08 \times 10^{-9} \text{ m}^2 \text{ s}^{-1}.$$

Solution

The equilibrium concentration of oxygen at the surface of the bubble:

$$x_s = (1.01325 \times 10^5)(0.21)/(4.052 \times 10^9) = 5.25 \times 10^{-6} [-]$$

Exposure time of the bubble:

$$t_c = (0.5)/(2.0) = 0.25 \text{ s}$$

Molar density of the bulk liquid:

$$c = (1000)/(18.02) = 55.5 \text{ kmol m}^{-3}$$

Mass transfer coefficient according to Eq.

$$\begin{aligned} k_L &= (2)\sqrt{(2.08 \times 10^{-9})/(3.14)(0.25)} \\ &= 1.0 \times 10^{-4} \text{ m s}^{-1} \end{aligned}$$

Rate of mass transfer:

$$N_A = (55.5)(1.0 \times 10^{-4})(5.25 \times 10^{-6}) \\ = 2.31 \times 10^{-8} \text{ kmol m}^{-2} \text{ s}^{-1}$$

Surface area of the bubble:

$$A = (3.14)(3 \times 10^{-3})^2 = 2.86 \times 10^{-5} \text{ m}^2$$

Amount of oxygen absorbed by the single bubble during the rising period:

$$R = (2.31 \times 10^{-8})(2.86 \times 10^{-5})(0.25) \\ = 1.65 \times 10^{-10} \text{ [mol/bubble]}$$