

Fundamental of Mass Transfer

By

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Your objectives in studying this section are to be able to: 1- Convert a composition given in mass fraction to mole fraction, and the reverse.

2- Transform a material from one measure of concentration to another, including mass/volume and moles/volume.

# Definition of mass transfer:

#### Mass transfer

 Mass transfer is mass in transit as the result of a species concentration difference in a mixture. A species concentration gradient in a mixture provides the driving potential for transport of that species.

#### What is the meaning of species?

 A species may be a single atom or a complex poly-atomic molecule. It can also be appropriate to identify a mixture (such as air) as a species.

# Example of Mass Transfer in Chemical Engineering Processes





# Analogy between heat and mass transfer

We can develop an understanding of mass transfer in a short time with little effort by simply drawing parallels between heat and mass transfer.

#### Temperature

- Both heat and mass are transferred from the more concentrated regions to the less concentrated ones.
- If there is no difference between the concentrations of a species at different parts of a medium, there will be no mass transfer.





## Convection

Mass convection (or *convective mass transfer*) is the mass transfer mechanism between a surface and a moving fluid that involves both *mass diffusion* and *bulk fluid motion*.

Fluid motion also enhances mass transfer considerably.

 $\dot{m}_{\rm conv} = h_{\rm mass} A_s (C_s - C_{\infty})$  Rate of mass convection

 $h_{\text{mass}}$  the mass transfer coefficient  $A_{\text{s}}$  the surface area  $C_{\text{s}} = C_{\text{s}}$  a suitable concentration dif

 $C_s - C_{\infty}$  a suitable concentration difference across the concentration boundary layer.

# Mass Transfer Theories

Velocities and Fluxes

# Your objectives in studying this section are to be able to:

 Define the following terms: mass-average velocity, molaraverage velocity, mass (or molar) flux, and diffusion mass (or molar) flux. 2- Write down an expression to calculate the mass (or molar) flux relative to a fixed coordinate system in terms of the diffusion mass (or molar) flux and the bulk motion contribution.

### Mass diffusion

Fick's law of diffusion states that the rate of diffusion of a chemical species at a location in a gas mixture (or liquid or solid solution) is proportional to the *concentration gradient* of that species at that location.

#### 1 Mass Basis

On a *mass basis,* concentration is expressed in terms of density (or *mass concentration*).

$$v = \frac{\sum_{i=1}^{n} \rho_i v_i}{\sum_{i=1}^{n} \rho_i} = \frac{\sum_{i=1}^{n} \rho_i v_i}{\rho} = \sum_{i=1}^{n} \omega_i v_i$$

Partial density of species i: Total density of mixture:  $\rho_i = m_i / V \qquad (kg/m^3)$  $\rho = m / V = \sum m_i / V = \sum \rho_i$ 



The *density of a mixture* at a location is equal to the sum of the *densities of its constituents* at that location.

Mass fraction of species i:

$$w_i = \frac{m_i}{m} = \frac{m_i/V}{m/V} = \frac{\rho_i}{\rho}$$

# 2 Mole Basis

On a *mole basis,* concentration is expressed in terms of molar concentration (or *molar density*), which is the amount of matter in kmol per unit volume.

Partial molar concentration of species i: $C_i = N_i/V$  (kmol/m³)Total molar concentration of mixture: $C = N/V = \sum N_i/V = \sum C_i$ 

Mole fraction of species i:

$$y_i = \frac{N_i}{N} = \frac{N_i/V}{N/V} = \frac{C_i}{C}$$

Again the mole fraction of a species ranges between 0 and 1, and the sum of the mole fractions of the constituents of a mixture is unity,  $\sum y_i = 1$ .

$$C_{i} = \frac{\rho_{i}}{M_{i}} \text{ (for species i)} \quad \text{and} \quad C = \frac{\rho}{M} \quad \text{(for the mixture)}$$
$$M = \frac{m}{N} = \frac{\sum N_{i}M_{i}}{N} = \sum \frac{N_{i}}{N} M_{i} = \sum y_{i}M_{i} \quad w_{i} = \frac{\rho_{i}}{\rho} = \frac{C_{i}M_{i}}{CM} = y_{i}\frac{M_{i}}{M}$$

How the mass and no. of mole are related to each other?

$$C_{i} = \frac{P_{i}}{M_{i}} \text{ and } C = \frac{P}{M}$$

$$Molecular weight of the mixture = M = \frac{M}{M} = \frac{\sum N:M}{M} = \sum Y_{i}M_{i}$$

The mass and mole Fraction :-  

$$w_i = \frac{p_i}{p} = \frac{c_i M_i}{c_i M_i} = y_i \frac{M_i}{M_i}$$

# Special Case: Ideal Gas Mixtures

At low pressures, a gas or gas mixture can conveniently be approximated as an ideal gas with negligible error.

The total pressure of a gas mixture P is equal to the sum of the partial pressures  $P_i$  of the individual gases in the mixture..

Here  $P_i$  is called the partial pressure of species *i*, which is the pressure species *i* would exert if it existed alone at the mixture temperature and volume (Dalton's law of additive pressures).

Then using the ideal gas relation  $PV = NR_u T$  where  $R_u$  is the universal gas constant for both the species *i* and the mixture, the pressure fraction of species *i* can be expressed as

$$\frac{P_i}{P} = \frac{N_i R_u T/V}{N R_u T/V} = \frac{N_i}{N} = y_i$$

The *pressure fraction* of species *i* of an ideal gas mixture is equivalent to the *mole fraction* of that species and can be used in place of it in mass transfer analysis.



A mixture of two ideal gases A and B

$$y_A = \frac{N_A}{N} = \frac{2}{2+6} = 0.25$$

 $P_A = y_A P = 0.25 \times 120 = 30$  kPa

**Press** we and mole fractions when we have ideal g

The composition of dry standard atmosphere is given on molar basis to be 78.1 % N2, 20.9 % O2 and 1.0 percent Ar and small amounts of other constituents. Treating other constituents as Ar, determine the mass fraction of the constituents of Air.

The molar masses again is determined to be: 
$$M = \sum_{i} M_i = 0.781 \times 28 + 0.209 \times 32 + 39.9 \times 0.01$$
  
= 29.0 kg/kmol  
Muss fraction:

$$w_{M_2} = y_i \frac{M_i}{M} = 0.781 \times \frac{28^{-cg/kmol}}{29 kg/kmol} = 0.754$$

$$W_{0_2} = y_{0_2} + \frac{M_{0_2}}{M} = 0.209 + \frac{32}{29} = 0.231$$

$$W_{Ar} = Y_{Ar} # \frac{M_{Ar}}{M} = 0.01 + \frac{39.9}{29} = 0.014$$

The composition of dry standard atmosphere is given on molar basis to be 77.9 % N2, 20.3 % O2 and 1.0 percent Ar and small amounts of other constituents. Treating other constituents as Ar, determine the mass fraction of the constituents of Air.

Determine the mole fraction of the water vapor at the surface of a lake whose temperature is 15 °C and compare it to the mole fraction of water in the lake. Take the atmospheric pressure at lake level to be 92 kPa

air and vapor to be ideal gas  
So the mole fraction of water vapor = 
$$\frac{P_i}{P} = \frac{1-705}{92} = 0.0185$$

# What is the meaning of mass or molar fluxes?

The mass (or molar)flux of a given species is a vector quantity denoting the amount of the particular species, in either mass or molar units, that passes per given unit time through a unit area normal to the vector.

The flux may be defined with reference

- 1- to coordinates that are fixed in space,
- 2- coordinates which are moving with the mass-average velocity, or

3- coordinates which are moving with the molar-average velocity

The mass flux of species i with respect to coordinates that are fixed in space is defined by

 $n_i = \rho_i v_i$ 

If we sum the component fluxes, we obtain the total mass flux,

 $n = \rho v$ 

The molar flux of species i with respect to coordinates that are fixed in space is given by

 $N_i = c_i v_i$ 

The **total molar flux** is the sum of these quantities:

#### Fick's Law of Diffusion: Stationary Medium Consisting of Two Species

kmol/s·m<sup>2</sup>).

Mass flux = Constant of proportionality  $\times$  Concentration gradient Fick's law of diffusion

Mass basis: 
$$j_{\text{diff},A} = \frac{\dot{m}_{\text{diff},A}}{A} = -CD_{AB}\frac{d(\rho_A/\rho)}{dx} = -CD_{AB}\frac{dw_A}{dx}(\text{kg/s}\cdot\text{m}^2)$$
  
Mole basis:  $\bar{j}_{\text{diff},A} = \frac{\dot{N}_{\text{diff},A}}{A} = -CD_{AB}\frac{d(C_A/C)}{dx} = -CD_{AB}\frac{dy_A}{dx}(\text{kmol/s}\cdot\text{m}^2)$   
Mass basis ( $\rho = \text{constant}$ ):  $j_{\text{diff},A} = -D_{AB}\frac{dr_A}{dx}$  (kg/s·m<sup>2</sup>)  
Mole basis ( $C = \text{constant}$ ):  $\bar{j}_{\text{diff},A} = -D_{AB}\frac{dC_A}{dx}$  (kmol/s·m<sup>2</sup>)  
Here  $j_{\text{diff},A}$  is the (diffusive)  
mass flux of species A (mass  
transfer by diffusion per unit  
time and per unit area normal  
to the direction of mass  
transfer, in kg/s·m<sup>2</sup>) and  $\bar{j}_{\text{diff},A}$   
is the (diffusive) molar flux (in  
FIGURE 14–10  
Higher concentration  
of species A  
Higher concentration  
of species A  
(kmol/s·m<sup>2</sup>)  
Here  $j_{\text{diff},A}$  is the (diffusive)  
mass flux of species A (mass  
transfer, in kg/s·m<sup>2</sup>) and  $\bar{j}_{\text{diff},A}$   
FIGURE 14–10

Various expressions of Fick's law of diffusion for a binary mixture.

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# Fick's Law of Diffusion

$$\frac{\delta^2 C_A}{\delta x^2} + \frac{\delta^2 C_A}{\delta y^2} + \frac{\delta^2 C_A}{\delta z^2} = \frac{1}{D} \frac{\delta C_A}{d\tau}$$

The rate equation for mass diffusion is known as Fick's law, and for transfer of species A in a binary mixture of A and B, it may express in vector form as:

$$j_A = -
ho D_{AB} 
abla m_A \qquad rac{kg}{s.m^2}$$

The Fick's law can be stated as:

$$N_A = -D_{AB} \frac{dC_a}{dx}$$

Mass Fly: Constant of Provision Mass Fly: Constant of Provision X Gong adject Mass Basis =  $-p P_{AB} \frac{d(P_{A}/p)}{dx} = -p P_{AB} \frac{\partial w_{A}}{\partial x}$ . mole Basis =  $-(D_{AB} \frac{d(P_{A}/p)}{dx}) = -(D_{AB} \frac{\partial w_{A}}{\partial x})$ The species flux may also be evaluated on a molar basis

$$J_A = -CD_{AB} \nabla x_A$$

## What is the meaning of mass or molar fluxes?

The mass flux of species i with respect to coordinates that are fixed in space is defined by:

 $n_i = \rho_i v_i$ 

If we sum the component fluxes, we obtain *the total mass flux*,

 $n = \rho v$ 

The molar flux of species i with respect to coordinates that are fixed in space is given by

The mass diffusion flux of species i with respect to the massaverage velocity is given by

$$j_i = \rho_i(v_i - v)$$
 and  $\sum_{i=1}^n j_i = 0$ 

The molar diffusion flux of species i with respect to the molaraverage velocity is given by

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$$J_i = c_i(v_i - V)$$
 and  $\sum_{i=1}^{n} J_i = 0$ 

 $N_i = c_i v_i$ 

The **total molar flux** is the sum of these quantities:

N = cV

# Mass and Molar diffusion fluxes:

The mass flux  $n_i$  is related to the mass diffusion flux as

$$n_i = j_i + \rho_i v = j_i + \omega_i n$$

The molar flux  $N_i$  is related to the molar diffusion flux as

$$N_i = J_i + c_i V = J_i + y_i N$$

### Mass Diffusivity

Fick's law defines a second important transport property, coefficient or mass diffusivity, D<sub>AB</sub>. namely, the binary diffusion

Its fundamental dimensions are obtained from:

$$D_{AB} = \left(\frac{M}{L^2 t}\right) \left(\frac{1}{M/L^3 \cdot 1/L}\right) = \frac{L^2}{t}$$

 $D_{AB}$  for the binary mixture of two gases, A and B has been given considerable attention for predicting  $D_{AB}$ :

- Because molecular velocities increase with rise of temperature T, so the diffusivity will increase. For gas, the diffusivity is proportional to T<sup>1.5</sup>.

- As the pressure P increases, the molecules become closer together and the mean free path is shorter and consequently the diffusivity is reduced. so, diffusivity for a gas becoming approximately inversely proportional to the pressure.

 $D_{AB} \propto T^{1.5}/P$ 

$$D_{AB} \propto \frac{T^{3/2}}{P}$$
 or  $\frac{D_{AB,1}}{D_{AB,2}} = \frac{P_2}{P_1} \left(\frac{T_1}{T_2}\right)^{3/2}$ 

$$D_{AB} \approx \frac{1}{3} \bar{c} \lambda_{mfp} \sim P^{-1} T^{3/2}$$

#### T= Absolute temperature in Kelvin

 $\bar{c}$ = the mean electron velocity, which increases with increasing the temperature and decreasing molecular weight and therefore the mass diffusivity increases with increasing the temperature and molecular weight.

 $\lambda_{mfp}$  = the electron mean free path, which is inversely proportional to gas pressure, so the mass diffusivity decreases with increasing pressure.

#### TABLE 14-1

Binary diffusion coefficients of some gases in air at 1 atm pressure (from Mills, 1995; Table A.17a, p. 869)

#### Binary Diffusion Coefficient,\* $m^2/s \times 10^5$

<i>T</i> , K	02	$CO_2$	$H_2$	NO	
200	0.95	0.74	3.75	0.88	
300	1.88	1.57	7.77	1.80	
400	5.25	2.63	12.5	3.03	
500	4.75	3.85	17.1	4.43	
600	6.46	5.37	24.4	6.03	
700	8.38	6.84	31.7	7.82	
800	10.5	8.57	39.3	9.78	
900	12.6	10.5	47.7	11.8	
1000	15.2	12.4	56.9	14.1	
1200	20.6	16.9	77.7	19.2	
1400	26.6	21.7	99.0	24.5	
1600	33.2	27.5	125	30.4	
1800	40.3	32.8	152	37.0	
2000	48.0	39.4	180	44.8	

TABLE	E 14-3	

Binary diffusion coefficients of dilute liquid solutions and solid solutions at 1 atm (from Barrer, 1941; Reid et al., 1977; Thomas, 1991; and van Black, 1980)

(a) Diffusion through Liquids			(b) Diffusion through Solids				
Substance A (Solute)	Substance <i>B</i> (Solvent)	<i>Т,</i> К	<i>D<sub>AB</sub></i> , m <sup>2</sup> /s	Substance A (Solute)	Substance <i>B</i> (Solvent)	<i>Т</i> , К	D <sub>AB</sub>
Ammonia Benzene Carbon dioxide Chlorine Ethanol Ethanol Ethanol Glucose Hydrogen	Water Water Water Water Water Water Water Water Water Water	285 293 298 285 283 288 298 298 298 298	$\begin{array}{c} D_{AB}, 1113\\ \hline 1.6 \times 10^{-9}\\ 1.0 \times 10^{-9}\\ 2.0 \times 10^{-9}\\ 1.4 \times 10^{-9}\\ 0.84 \times 10^{-9}\\ 1.0 \times 10^{-9}\\ 1.2 \times 10^{-9}\\ 0.69 \times 10^{-9}\\ 6.3 \times 10^{-9} \end{array}$	Carbon dioxide Nitrogen Oxygen Helium Helium Hydrogen Hydrogen	Natural rubber Natural rubber Natural rubber Pyrex Pyrex Silicon dioxide Iron Nickel Nickel	298 298 298 773 293 298 298 358 438	1.1 > 1.5 > 2.1 > 2.0 > 4.5 > 4.0 > 2.6 > 1.2 > 1.0 >
Methane Methane Methane Methanol Nitrogen Oxygen Water Water Water Chloroform	Water Water Water Water Water Ethanol Ethylene glycol Methanol	298 275 293 333 288 298 298 298 298 298 298 298	$\begin{array}{c} 0.3 \times 10 \\ 0.85 \times 10^{-9} \\ 1.5 \times 10^{-9} \\ 3.6 \times 10^{-9} \\ 1.3 \times 10^{-9} \\ 2.6 \times 10^{-9} \\ 2.4 \times 10^{-9} \\ 1.2 \times 10^{-9} \\ 1.2 \times 10^{-9} \\ 1.8 \times 10^{-9} \\ 1.8 \times 10^{-9} \\ 2.1 \times 10^{-9} \end{array}$	Cadmium Zinc Zinc Antimony Bismuth Mercury Copper Copper Carbon Carbon	Copper Copper Copper Silver Lead Lead Aluminum Aluminum Iron (fcc) Iron (fcc)	293 773 1273 293 293 293 773 1273 773 1273	1.0 × 2.7 × 4.0 × 5.0 × 3.5 × 1.1 × 2.5 × 4.0 × 1.0 × 5.0 × 3.0 ×

1. The diffusion coefficients, in general, are *highest in gases* and *lowest in solids*. The diffusion coefficients of gases are several orders of magnitude greater than those of liquids.

2. Diffusion coefficients *increase with temperature*. The diffusion coefficient (and thus the mass diffusion rate) of carbon through iron during a hardening process, for example, increases by 6000 times as the temperature is raised from 500°C to 1000°C.

#### TABLE 14-4

m²/s  $10^{-10}$  $10^{-10}$  $10^{-10}$  $10^{-12}$  $10^{-15}$  $10^{-14}$  $10^{-13}$  $10^{-12}$  $10^{-11}$  $10^{-19}$  $10^{-18}$  $10^{-13}$  $10^{-25}$  $10^{-20}$  $10^{-19}$  $10^{-14}$  $10^{-10}$  $10^{-15}$  $10^{-11}$  In a binary ideal gas mixture of species A and B, the diffusion coefficient of A in B is equal to the diffusion coefficient of B in A, and both increase with temperature

<i>T</i> , ℃	D <sub>H2O-Air</sub> or D <sub>Air-H2O</sub> at 1 atm, in m <sup>2</sup> /s (from Eq. 14–15)
0	$2.09 \times 10^{-5}$
5	$2.17 \times 10^{-5}$
10	$2.25 \times 10^{-5}$
15	$2.33 \times 10^{-5}$
20	$2.42 \times 10^{-5}$
25	$2.50 \times 10^{-5}$
30	$2.59 \times 10^{-5}$
35	$2.68 \times 10^{-5}$
40	$2.77 \times 10^{-5}$
50	$2.96 \times 10^{-5}$
100	$3.99 \times 10^{-5}$
150	$5.18 \times 10^{-5}$

$$D_{AB} = D_{BA}$$

The value of  $D_{AB}$  for certain combinations of components are available in literature. It can be proved that  $D_{AB} = D_{BA}$ . When one molecule of A moves in the x direction, one molecule of B has to move in the opposite direction. Otherwise, a macroscopic density gradient will develop, which is not sustainable, (A is area)

$$N_A/A = -D_{AB}\frac{dC_A}{dx}$$

$$A = -D_{BA}\frac{dC_B}{dx} = -D_{BA}\frac{d(1-C_A)}{dx} = D_{BA}\frac{dC_A}{dx}$$

$$N_A/A = -N_B/A$$

$$D_{AB} = D_{BA}$$

 $N_{R}$ 

#### Conservation of species for a control volume

The rate at which the mass of some species enters a control volume, plus the rate at which the species mass is generated within the control volume, minus the rate at which this species mass leaves the control volume must equal the rate of increase of the species mass stored within the control volume.



Figure 2.1: Conservation of species for a control volume.

$$\hat{M}_{A,in} + \hat{M}_{A,g} - \hat{M}_{A,out} = \frac{dM_A}{dt} \equiv \hat{M}_{A,st}$$

#### The Mass Diffusion Equation:

$$n_{a,x+dx}dydz = n_{a,x}dydz + \frac{\partial[n_{a,x}dydz]}{\partial x}dx$$

$$n_{a,y+dy}dxdz = n_{a,y}dxdz + \frac{\partial[n_{a,y}dxdz]}{\partial x}dy$$

$$n_{a,z+dz}dxdy = n_{a,z}dxdy + \frac{\partial [n_{a,z}dxdy]}{\partial x}dz$$



# Adding Terms to Mass diffusion Equation

- May be volumetric chemical reaction occurring through out the medium perhaps non-uniformly.
- The rate at which species A is generated within the control volume due to such reactions may be expressed as

where  $n_A$  is the rate of increase of the mass of species A per unit volume of the mixture (kg  $\cdot$  s  $^{-1} \cdot$  m<sup>-3</sup>).

- A stored within the control volume, and the rate of change is:

$$\dot{M}_{A,st} = \frac{\partial \rho_A}{\partial t} \, dx \, dy \, dz$$

 $\dot{M}_{A,q} = \dot{n}_A \, dx \, dy \, dz$ 

### **Conservation Equation**

$$-\frac{\partial n_A}{\partial x} - \frac{\partial n_A}{\partial y} - \frac{\partial n_A}{\partial z} + \dot{n}_A = \frac{\partial \rho_A}{\partial t}$$

Then, substituting the x, y, and z components of Equation, we obtain

$$\frac{\partial}{\partial x}(\rho D_{AB}\frac{\partial \omega_A}{\partial x}) + \frac{\partial}{\partial y}(\rho D_{AB}\frac{\partial \omega_A}{\partial y}) + \frac{\partial}{\partial z}(\rho D_{AB}\frac{\partial \omega_A}{\partial z}) + \dot{n}_A = \frac{\partial \rho_A}{\partial t}$$

In terms of the molar concentration, a similar derivation yields

$$\frac{\partial}{\partial x}(CD_{AB}\frac{\partial x_A}{\partial x}) + \frac{\partial}{\partial y}(CD_{AB}\frac{\partial x_A}{\partial y}) + \frac{\partial}{\partial z}(CD_{AB}\frac{\partial x_A}{\partial z}) + \dot{N}_A = \frac{\partial C_A}{\partial t}$$

# Simplifying Conservation Equation ....

• Simplified equation of the foregoing equations can be written as follows if  $D_{AB}$  and  $\rho$  are constant:

$$\frac{\partial^2 \rho_A}{\partial x^2} + \frac{\partial^2 \rho_A}{\partial y^2} + \frac{\partial^2 \rho_A}{\partial z^2} + \frac{\dot{n}_A}{D_{AB}} = \frac{1}{D_{AB}} \frac{\partial \rho_A}{\partial t}$$

• Similarly, if  $D_{AB}$  and c are constant, Equations can be simplified as follows:

$$\frac{\partial^2 c_A}{\partial x^2} + \frac{\partial^2 c_A}{\partial y^2} + \frac{\partial^2 c_A}{\partial z^2} + \frac{\dot{N}_A}{D_{AB}} = \frac{1}{D_{AB}} \frac{\partial c_A}{\partial t}$$

### Other geometry for Conservation Equations:

• Cylindrical Coordinates:

$$\frac{1}{r}\frac{\partial}{\partial r}(cD_{AB}r\frac{\partial x_A}{\partial r}) + \frac{1}{r^2}\frac{\partial}{\partial \phi}(cD_{AB}\frac{\partial x_A}{\partial \phi}) + \frac{\partial}{\partial z}(cD_{AB}\frac{\partial x_A}{\partial z}) + \dot{N}_A = \frac{\partial c_A}{\partial t}$$

• Spherical Coordinates:

$$\frac{1}{r^2}\frac{\partial}{\partial r}(cD_{AB}r^2\frac{\partial x_A}{\partial r}) + \frac{1}{r^2sin^2\theta}\frac{\partial}{\partial \phi}(cD_{AB}\frac{\partial x_A}{\partial \phi}) + \frac{1}{r^2sin\theta}\frac{\partial}{\partial \theta}(cD_{AB}sin\theta)\frac{\partial x_A}{\partial \theta} + \dot{N}_A = \frac{\partial c_A}{\partial t}$$

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# Mass Transfer Theories

Assignment 1



 Beginning with a differential control volume, derive the diffusion equation, on a molar basis, for species A in a three-dimensional (Cartesian coordinates), stationary medium, considering species generation with constant properties.



Consider the radial diffusion of a gaseous species (A) through the wall of a plastic tube (B), and allow for chemical reactions that provide for the depletion of A at a rate N<sup>•</sup> A (kmol · s <sup>-1</sup> · m<sup>-3</sup>). Derive a differential equation that governs the molar concentration of species A in the plastic.

- The pressure in a pipeline that transports helium gas at a rate of 2 kg/s is maintained at 1 atm by venting helium to the atmosphere through a 5-mminternal-diameter tube that extends 15 m into the air as shown in figure beside. Assuming both the helium and the atmospheric air to be 25 oC, determine:
- A- the mass flowrate of helium lost to the atmosphere through the tube.
- B- the mass flowrate that infiltrates into the pipeline
- C- the flow velocity at the bottom of the tube where it is attached to the pipeline that will be measured by an anemometer in steady operation
## Problem 1.4

• A thin plastic membrane is used to separate helium from a gas stream. Under steady-state conditions the concentration of helium in the membrane is known to be 0.02 and 0.005 kmol  $\cdot$  m<sup>-3</sup> at the inner and outer surfaces, respectively. If the membrane is 1 mm thick and the binary diffusion coefficient of helium with respect to the plastic is  $10^{-9}m^2 \cdot s^{-1}$ , what is the diffusive flux?

# **Boundary Conditions**

Lecture 3

# Types of Diffusion

Ordinary diffusion: The primary driving mechanism of mass diffusion is the concentration gradient, and mass diffusion due to a concentration gradient is known as the ordinary diffusion.

Temperature gradients in a medium can cause thermal diffusion (also called the soret effect), and pressure gradients may result in pressure diffusion.

Forced diffusion: An external force field such as an electric or magnetic field applied on a mixture or solution can be used successfully to separate electrically charged or magnetized molecules (as in an electrolyte or ionized gas) from the mixture.

Knudsen diffusion: When the pores of a porous solid such as silica-gel are smaller than the mean free path of the gas molecules, the molecular collisions may be negligible and a free molecule flow may be initiated.

Surface diffusion: When the size of the gas molecules is comparable to the pore size, adsorbed molecules move along the pore walls.

Brownian motion: Particles whose diameter is under 0.1 m such as mist and soot particles act like large molecules, and the diffusion process of such particles due to the concentration gradient is called Brownian motion.

# **Boundary Conditions**

• For a surface at x = 0, the constant surface species concentration boundary condition is expressed as:

 $C_{\rm A}(0,t) = C_{{\rm A},s}$ 

 $x_{\mathrm{A}}(0,t) = x_{\mathrm{A},s}$ 

To take a familiar example, consider a pool of water that is exposed to air. If we are interested in determining the rate at which water vapor is transferred into the air, we would need to specify the water vapor concentration in the air at the air–water interface.

# Evaporation and Sublimation

A common mass transfer scenario is the transfer of a species A into a gas stream due to evaporation or sublimation from a liquid or solid surface, respectively (Figure beside). Conditions within the gas phase are of interest, and the concentration (or partial pressure) of species A in the gas phase at the interface (located at x =0) may readily be determined from Raoult's law:

 $p_{\rm A}(0) = x_{\rm A}(0)p_{\rm A,sat}$ 

- Raoult's law applies if the gas phase can be approximated as ideal and the liquid or solid phase has a high concentration of species A.
- If the liquid or solid is a pure species A, that is,  $x_A = 1$ , Equation simplifies to  $p_A(0) = p_A$ , sat. That is, the partial pressure of the vapor at the interface corresponds to saturated conditions at the temperature of the interface and may be determined from standard thermodynamic tables.



# **Boundary Conditions**

con Unlike temperature the the two ation of ature or (solid sides of species on solid sas of solecies on solid light as on under ature solid sides of solecies on solid light as on under ature solid sol (1) *specified species concentration,* which corresponds to specified temperature (2) specified species flux, which corresponds to specified heat flux.

interrace are usually not

 $\dot{y}_{H_2O,liquid side} \cong 1.0$ 



• Solubility: The maximum amount of solid that can be dissolved in a liquid at a specified temperature.

$$w_{\text{salt, liquid side}} = \frac{m_{\text{salt}}}{m} = \frac{36.5 \text{ kg}}{(100 + 36.5) \text{ kg}} = 0.267$$

(or 26.7 percent)

 $P_{i, \text{ gas side}} \propto P y_{i, \text{ liquid side}}$ 

 $y_{i, \text{ gas side}} \propto y_{i, i}$ 

 $y_{i, \text{ gas side}} = P_{i, \text{ gas side}}/P$ 

• Henry's constant *H*: The product of the total pressure of the gas mixture and the proportionality constant.

$$y_{i, \text{ liquid side}} = \frac{P_{i, \text{ gas side}}}{H} (\text{at interface})$$

# Solubility and Henry's constant.

#### TABLE 14-5

Solubility of two inorganic compounds in water at various temperatures, in kg, in 100 kg of water [from *Handbook of Chemistry* (New York: McGraw-Hill, 1961)]

		Solute					
Tempera- ture, K	Salt, NaCl	Calcium Bicarbonate, Ca(HCO <sub>3</sub> ) <sub>2</sub>					
273.15	35.7	16.15					
280	35.8	16.30					
290	35.9	16.53					
300	36.2	16.75					
310	36.5	16.98					
320	36.9	17.20					
330	37.2	17.43					
340	37.6	17.65					
350	38.2	17.88					
360	38.8	18.10					
370	39.5	18.33					
373.15	39.8	18.40					

#### TABLE 14-6

Henry's constant *H* (in bars) for selected gases in water at low to moderate pressures (for gas i,  $H = P_{i, \text{ gas side}}/y_{i, \text{ water side}}$ ) (from Mills, 1995; Table A.21)

Solute	290 K	300 K	310 K	320 K	330 K	340 K
H <sub>2</sub> S	440	560	700	830	980	1140
$CO_2$	1280	1710	2170	2720	3220	_
02	38,000	45,000	52,000	57,000	61,000	65,000
$H_2$	67,000	72,000	75,000	76,000	77,000	76,000
CO	51,000	60,000	67,000	74,000	80,000	84,000
Air	62,000	74,000	84,000	92,000	99,000	104,000
$N_2$	76,000	89,000	101,000	110,000	118,000	124,000

# Solubility of Gases in Liquids and Solids

- Another common scenario is mass transfer of species A from a gas phase into a liquid or solid, species B (Figure Beside ). Mass transfer within the liquid or solid phase is of interest, and the concentration of species A at the interface is required as a boundary condition.
- If species A is only weakly soluble (x<sub>A</sub> is small) in a liquid, Henry's law may be used to relate the mole fraction of A in the liquid to the partial pressure of A in the gas phase outside the liquid:



- 1. The concentration of a gas dissolved in a liquid is inversely proportional to Henry's constant. The larger the Henry's constant, the smaller the concentration of dissolved gases in the liquid.
- 2. Henry's constant increases (and thus the fraction of a dissolved gas in the liquid decreases) with increasing temperature. Therefore, the dissolved gases in a liquid can be driven off by heating the liquid.
- 3. The concentration of a gas dissolved in a liquid is proportional to the partial pressure of the gas. The amount of gas dissolved in a liquid can be increased by increasing the pressure of the gas. This can be used to advantage in the carbonation of soft drinks with CO<sub>2</sub> gas.

Henry's constant <i>H</i> (in bars) for selected gases in water at low to moderate pressures (for gas <i>i</i> , $H = P_{i, \text{ gas side}}/y_{i, \text{ water side}}$ ) (from Mills, 1995; Table A.21)									
Solute	290 K	300 K	310 K	320 K	330 K	340 K			
$H_2S$	440	560	700	830	980	1140			
$CO_2$	1280	1710	2170	2720	3220				
O2	38,000	45,000	52,000	57,000	61,000	65,000			
$H_2$	67,000	72,000	75,000	76,000	77,000	76,000			
CO	51,000	60,000	67,000	74,000	80,000	84,000			
Air	62,000	74,000	84,000	92,000	99,000	104,000			
$N_2$	76,000	89,000	101,000	110,000	118,000	124,000			





or



or

 $P_{A,\text{gas side}} = H y_{A,\text{liquid side}}$ 

# Problem 1.4

• Determine the mole fraction of air dissolved in water at the surface of the lake whose temperature is 17 oC. Take the atmospheric pressure at lake level to be 92 kPa.

The mole fraction of air dissolved in water at the surface of the lake is to be determined.  
Assumption: I - Both water and Vapor are idealgases.  
2 - Air is weakly soluble in water so that Henry's law is applicable  
Properties: - The sut. Pressure of water at 17 °C is 1.96 kpc  
Henry's Constant for air dissolved in Waterat 290k is H = 62,000 bar.  
Propor = Psut = 1.96  
P= Panyair + Prapor , Paryair = P- Prapor => Paryair = 92-196 = 90.04 kpa  
Yair = 
$$\frac{0.9004}{0.000} = 1.45 \pm 10^{5}$$

Solubility : The maximum amount of solid that can be dissolved in a liquid at a specified temperature.

# Gas-Solid interface

- Conditions at a gas—solid interface may also be determined if the gas, species A, dissolves in a solid, species B, and a solution is formed. In such cases mass transfer in the solid is independent of the structure of the solid and may be treated as a diffusion process.
- Treating the gas and solid as a solution, we can obtain the concentration of the gas in the solid at the interface through use of a property known as the solubility, S. It is defined by the expression:



$$C_{\rm A}(0) = Sp_{\rm A}(0)$$

# Problem 1.3 Diffusion of Hydrogen Gas into Nickel Plate

• Consider a nickel plate that is in contact with hydrogen gas at 358 K and 300 kPa. Determine the molar and mass density of hydrogen in the nickel at the interface.

Hydrogen gas is maintained at 3 bars and 1 bar on opposite sides of a plastic membrane, which is 0.3 mm thick. The temperature is 25°C, and the binary diffusion coefficient of hydrogen in the plastic is 8.7 10<sup>-8</sup> m<sup>2</sup>/s. The solubility of hydrogen in the membrane is 1.5 × 10<sup>-3</sup> kmol/m<sup>3</sup> bar. What is the mass diffusive flux of hydrogen through the membrane?



# Mass Transfer Scenario

Lecture 5

Stationary Media with Specified Surface Concentrations :Plane wall

$$\frac{\partial^2 c_A}{\partial x^2} + \frac{\partial^2 c_A}{\partial y^2} + \frac{\partial^2 c_A}{\partial z^2} + \frac{\dot{N}_A}{D_{AB}} = \frac{1}{D_{AB}} \frac{\partial c_A}{\partial t}$$

Note:

- 1- No chemical reaction
- 2- Steady-state
- 3- one dimensional diffusion of species A through a planar medium of A, and B

$$\frac{d}{dx}(cD_{AB}\frac{dx_A}{dx}) = 0$$



$$N_{A,x} = -cD_{AB}\frac{x_{A,s_2} - x_{A,s_1}}{L}.$$

$$N_{A,x} = -D_{AB}A \frac{c_{A,s_2} - c_{A,s_1}}{L}.$$

$$R_{m,dif} = \frac{c_{A,s_1} - c_{A,s_2}}{N_{A,x}} = \frac{L}{D_{AB}}$$

#### STEADY MASS DIFFUSION THROUGH A WALL- Mass Basis

Many practical mass transfer problems involve the diffusion of a species through a plane-parallel medium that does not involve any homogeneous chemical reactions under *onedimensional steady* conditions.

$$\dot{m}_{\text{diff},A,\text{wall}} = \rho D_{AB} A \frac{w_{A,1} - w_{A,2}}{L} = D_{AB} A \frac{\rho_{A,1} - \rho_{A,2}}{L} \quad (\text{kg/s})$$

$$\dot{m}_{\text{diff, A, wall}} = \frac{w_{A, 1} - w_{A, 2}}{L/\rho D_{AB} A} = \frac{w_{A, 1} - w_{A, 2}}{R_{\text{diff, wall}}}$$

$$R_{\text{diff, wall}} = \frac{L}{\rho D_{AB} A} \qquad \begin{array}{c} \text{diffusion resistance of} \\ \text{the wall} \end{array}$$



The rate of mass diffusion through a plane wall is proportional to the average density, the wall area, and the concentration difference across the wall, but is inversely proportional to the wall thickness.

### STEADY MASS DIFFUSION THROUGH A WALL- Mole Basis

$$\dot{N}_{\text{diff, A, wall}} = CD_{AB}A \frac{y_{A,1} - y_{A,2}}{L} = D_{AB}A \frac{C_{A,1} - C_{A,2}}{L} = \frac{y_{A,1} - y_{A,2}}{\overline{R}_{\text{diff, wall}}}$$

 $\overline{R}_{\text{diff, wall}} = L/CD_{AB}A$ 

molar diffusion resistance of the wall in s/kmol



Stationary Media with Specified Surface Concentrations : Cylindrical coordinates

The analogy also applies to cylindrical and system.

$$\frac{1}{r}\frac{\partial}{\partial r}(cD_{AB}r\frac{\partial x_A}{\partial r}) + \frac{1}{r^2}\frac{\partial}{\partial \phi}(cD_{AB}\frac{\partial x_A}{\partial \phi}) + \frac{\partial}{\partial z}(cD_{AB}\frac{\partial x_A}{\partial z}) + \dot{N}_A = \frac{\partial c_A}{\partial t}$$

For the following condition:

1-one-dimensional,

2- steady diffusion in a cylindrical,

3- nonreacting medium,

Equation below:

$$\frac{d}{dr}(rcD_{AB}\frac{dx_A}{dr}) = 0$$



$$x_{\rm A}(r) = \frac{x_{\rm A,s1} - x_{\rm A,s2}}{\ln (r_1/r_2)} \ln \left(\frac{r}{r_2}\right) + x_{\rm A,s2}$$

$$R_{m,diff} = \frac{\ln(\frac{r_2}{r_1})}{2\pi L D_{AB}}$$

$$N_{A,r} = (C_{A,s1} - C_{A,s2})/R_{m,diff}$$



### Stationary Media with Specified Surface Concentrations :Spherical System



It will be reduced according to the following condition:

- 1- one-dimensional
- 2- steady-state

3-No reaction





$$x_{\rm A}(r) = \frac{x_{{\rm A},s1} - x_{{\rm A},s2}}{1/r_1 - 1/r_2} \left(\frac{1}{r} - \frac{1}{r_2}\right) + x_{{\rm A},s2}$$

$$Resistance = \frac{1}{4\pi D_{AB}} \left[\frac{1}{r_1} - \frac{1}{r_2}\right]$$

$$N_{A,r} = (C_{A,s1} - C_{A,s2})/R_{m,diff}$$

# Diffusion of Hydrogen through a spherical container

Pressurized hydrogen gas is stored at 358 K in a 4.8 m outer diameter spherical container made of nickel. The shell of the container is 6 cm thick. The molar concentration of hydrogen in the nickel at the inner surface is determined to be 0.087 kmol/m3. Thoncentration oh hydrogen in the nickel at the outer surface is negligible. Determine the mass flow rate of hydrogen diffusion through the nickel container.

OAssumption: - Omass diffusion is steady and one diemensional. 2 No chemical Reaction.

solution

 $C = C_{A+} C_{B}$ 



The container is stationary medium.  

$$M = 277.2207610$$

 Hydrogen stored in a vessel diffuses through the steel wall of 20 mm thickness. The molar concentration at the inner surface is 2 kg mol/m<sup>3</sup>. At the other surface it is zero. Assuming plane wall condition and D<sub>ab</sub> = 0.26 × 10<sup>-12</sup> m<sup>2</sup>/s, determine the mass of hydrogen diffused per 1 m<sup>2</sup>.



• Consider the diffusion of hydrogen (species A) in air, liquid water, or iron (species B) at T=293 K. Calculate the species flux on both molar and mass bases if the concentration gradient at a particular location is  $dC_A/dx = 1$ kmol/m<sup>3</sup>. m. Compare the value of the mass diffusivity to the thermal diffusivity. The mole fraction of the hydrogen,  $x_A$ , is much less than unity



• The efficacy of pharmaceutical products is reduced by prolonged exposure to high temperature, light, and humidity. For water vapor sensitive consumer products that are in tablet or capsule form and might be stored in humid environments such as bathroom medicine cabinets, blister packaging is used to limit the direct exposure of the medicine to humid conditions until immediately before its ingestion. Consider tablets that are contained in a blister package composed of a flat lidding sheet and a second, formed sheet that includes troughs to hold each tablet. The formed sheet is L= 50 micrometer thick and is fabricated of a polymer material. Each trough is of diameter D= 5 mm and depth h= 3 mm. The lidding sheet is fabricated of aluminum foil. The binary diffusion coefficient for water vapor in the polymer is  $D_{AB} = 6 \times 10^{-14} \text{ m}^2/\text{s}$  while the aluminum may be assumed to be impermeable to water vapor. For molar concentrations of water vapor in the polymer at the outer and inner surfaces of  $C_{A,s1}$ =4.5 ×10<sup>-3</sup> kmol/m<sup>3</sup> and  $C_{A,s2}$  =0.5× 10<sup>-3</sup> kmol/m<sup>3</sup>, respectively, determine the rate at which water vapor is transferred through the trough wall to the tablet.







# Diffusion of Vapor through a stationary gas: Stefan Flow

- Many engineering applications such as heat pipes, cooling ponds, and the familiar perspiration involve condensation, evaporation, and transpiration in the presence of a non-condensable gas, and thus the *diffusion* of a vapor through a stationary (or stagnant) gas.
- To understand and analyze such processes, consider a liquid layer of species *A* in a tank surrounded by a gas of species *B*, such as a layer of liquid water in a tank open to the atmospheric air at constant pressure *P* and temperature *T*.

$$\bar{j}_A = \dot{N}_A / A = \text{constant} \text{ (or } j_A = \dot{m}_A / A = \text{constant})$$

Noting that  $y_A + y_B = 1$  and that  $y_{A,0} > y_{A,L}$ , we must have  $y_{B,0} < y_{B,L}$ .

$$\bar{j}_B = \dot{N}_B / A = 0 \text{ (or } j_B = \dot{m}_B / A = 0)$$
$$\bar{j}_A = \dot{N}_A / A = \bar{j}_{A, \text{ conv}} + \bar{j}_{A, \text{ diff}} = y_A (\bar{j}_A + \bar{j}_B) - C D_{AB} \frac{dy_A}{dx}$$

$$\bar{j}_B = 0$$

$$\bar{j}_A = y_A \bar{j}_A - C D_{AB} \frac{dy_A}{dx}$$

$$\bar{j}_A = -\frac{CD_{AB}}{1 - y_A} \frac{dy_A}{dx} \longrightarrow -\frac{1}{1 - y_A} \frac{dy_A}{dx} = \frac{\bar{j}_A}{CD_{AB}} = \text{constant}$$
$$-\int_{A,0}^{y_{A,L}} \frac{dy_A}{1 - y_A} = \int_0^L \frac{\bar{j}_A}{CD_{AB}} dx \qquad \ln \frac{1 - y_{A,L}}{1 - y_{A,0}} = \frac{\bar{j}_A}{CD_{AB}} L$$

$$\bar{j}_A = \dot{N}_A / A = \frac{CD_{AB}}{L} \ln \frac{1 - y_{A,L}}{1 - y_{A,0}} \text{ (kmol/s·m^2)}$$

$$\dot{N}_{A} = \frac{D_{AB}P}{LR_{u}T} \ln \frac{P - P_{A,L}}{P - P_{A,0}} \text{ (kmol/s)}$$

This relation is known as Stefan's law, and the *induced convective flow* described that enhances mass diffusion is called the Stefan flow.



$$\ln \frac{1 - y_A}{1 - y_{A,0}} = \frac{\overline{j}_A}{CD_{AB}} x$$
$$\frac{1 - y_A}{1 - y_{A,0}} = \left(\frac{1 - y_{A,L}}{1 - y_{A,0}}\right)^{x/L}$$

# Equimolar Counter Diffusion

 $C = C_A + C_B = \text{constant}$  (kmol/m<sup>3</sup>)  $\dot{N}_A = -\dot{N}_B$  or  $\dot{N}_A + \dot{N}_B = 0$  (kmol/s)  $\dot{N} = \dot{N}_A + \dot{N}_B = 0 \longrightarrow CA\overline{V} = 0$  $\bar{j}_A = \dot{N}_A / A = -CD_{AB} \frac{dy_A}{dx}$  and  $\bar{j}_B = \dot{N}_B / A = -CD_{BA} \frac{dy_B}{dx}$  $\dot{N}_{\text{diff, A}} = CD_{AB}A \frac{y_{A,1} - y_{A,2}}{L} = D_{AB}A \frac{C_{A,1} - C_{A,2}}{L} = \frac{D_{AB}}{R}A \frac{P_{A,0} - P_{A,L}}{L}$  $\dot{N}_{\text{diff, }B} = CD_{BA}A \frac{y_{B,1} - y_{B,2}}{I} = D_{BA}A \frac{C_{B,1} - C_{B,2}}{I} = \frac{D_{BA}}{R_{A}T}A \frac{P_{B,0} - P_{B,L}}{L}$  $\dot{m} = \dot{m}_A + \dot{m}_B = \dot{N}_A M_A + \dot{N}_B M_B = \dot{N}_A (M_A + M_B)$   $\dot{N}_B = -\dot{N}_A$ 



Solubility: The maximum amount of solid that can be dissolved in a liquid at a specified temperature.

TABLE 14	-5		TABLE	14-6						
Solubility of two inorganic compounds in water at various temperatures, in kg, in 100 kg of			Henry's pressure <u>(from M</u>	constant <i>H</i> es (for gas <i>i</i> ills, 1995;	(in bars) fo , $H = P_{i, \text{ gas}}$ Table A.21)	r selected ga <sub>side</sub> /y <sub>i, water side</sub> )	ses in water )	at low to mo	derate	
water [from	Handboo	k of Chemistry	Solute	Solute 290 K 300 K 310 K 320 K 330 K 340 K						
(New York:	McGraw-F	lill, 1961)]	$H_2S$	440	560	700	830	980	1140	
		Solute	CO <sub>2</sub>	1280	1710	2170	2720	3220	—	
Tempera- ture, K	Salt, NaCl	Calcium Bicarbonate, Ca(HCO <sub>3</sub> ) <sub>2</sub>	O <sub>2</sub> H <sub>2</sub> CO Air	38,000 67,000 51,000 62,000	45,000 72,000 60,000 74,000	52,000 75,000 67,000 84,000	57,000 76,000 74,000 92,000	61,000 77,000 80,000 99,000	65,000 76,000 84,000 104,000	
273.15	35.7	16.15	N <sub>2</sub>	76,000	89,000	101,000	110,000	118,000	124,000	
280 290 300	35.8 35.9 36.2	16.30 16.53 16.75			$P_{i,i}$	$_{\rm gas\ side}$ $\propto$	P y <sub>i, liquid s</sub>	side		Gas phase includin species A $N''_{A,x}$ $p_A(C)$
320 330 240	36.9 37.2	17.20 17.43			Уi,	gas side =	P <sub>i, gas side</sub>	/ <i>P</i>		x Liquid or solid, species low concentration of
350 360 370 373,15	38.2 38.8 39.5 39.8	17.88 17.88 18.10 18.33 18.40		:	<i>Vi</i> , liquid si	$_{\rm de} = \frac{P_{i,\rm g}}{I}$	$\frac{1}{H}$ (at	interface	e)	( <i>b</i> )

Gas-liquid or gas-solid interface

		т	D
Substance A	Substance B	(K)	$D_{AB}$ $(m^2/s)$
Cases			
Gases		200	0.00
NH <sub>3</sub>	Air	298	$0.28 \times 10^{-4}$
$H_2O$	Air	298	$0.26 \times 10^{-4}$
CO <sub>2</sub>	Air	298	$0.16 \times 10^{-4}$
$H_2$	Air	298	$0.41 \times 10^{-4}$
O <sub>2</sub>	Air	298	$0.21 \times 10^{-4}$
Acetone	Air	273	$0.11  imes 10^{-4}$
Benzene	Air	298	$0.88  imes 10^{-5}$
Naphthalene	Air	300	$0.62  imes 10^{-5}$
Ar	$N_2$	293	$0.19  imes 10^{-4}$
H <sub>2</sub>	$O_2$	273	$0.70  imes 10^{-4}$
H <sub>2</sub>	$N_2$	273	$0.68  imes 10^{-4}$
H	$\overline{CO_2}$	273	$0.55  imes 10^{-4}$
CÔ <sub>2</sub>	Na	293	$0.16  imes 10^{-4}$
CO	$\Omega_2$	273	$0.14 \times 10^{-4}$
$O_2$	$N_2$	273	$0.18 imes10^{-4}$
Dilute Solutions			
Caffeine	H <sub>2</sub> O	298	$0.63 \times 10^{-9}$
Ethanol	H <sub>2</sub> O	298	$0.12 \times 10^{-8}$
Glucose	H <sub>2</sub> O	298	$0.69 \times 10^{-9}$
Glycerol	H <sub>2</sub> O	298	$0.94 \times 10^{-9}$
Acetone	H <sub>2</sub> O	298	$0.13 \times 10^{-8}$
CO		298	$0.20 \times 10^{-8}$
0	H-O	208	$0.20 \times 10^{-8}$
H	H_O	298	$0.24 \times 10^{-8}$
N <sub>2</sub>	H <sub>2</sub> O	298	$0.05 \times 10^{-8}$ $0.26 \times 10^{-8}$
1.2	1120	270	0.20 / 10
Solids			
O <sub>2</sub>	Rubber	298	$0.21 \times 10^{-9}$
N <sub>2</sub>	Rubber	298	$0.15  imes 10^{-9}$
CO <sub>2</sub>	Rubber	298	$0.11  imes 10^{-9}$
He	SiO <sub>2</sub>	293	$0.4  imes 10^{-13}$
H <sub>2</sub>	Fe	293	$0.26 \times 10^{-12}$
Cd	Cu	293	$0.27  imes 10^{-18}$
Al	Cu	293	$0.13 \times 10^{-33}$

 TABLE A.8
 Binary Diffusion Coefficients at One Atmosphere<sup>a,b</sup>

<sup>a</sup>Adapted with permission from References 24, 25, and 26.

<sup>b</sup>Assuming ideal gas behavior, the pressure and temperature dependence of the diffusion coefficient for a binary mixture of gases may be estimated from the relation

	$H = p_{\Lambda,i} / x_{\Lambda,i} \text{ (bars)}$							
Т (К)	NH <sub>3</sub>	Cl <sub>2</sub>	H <sub>2</sub> S	SO <sub>2</sub>	CO <sub>2</sub>	CH <sub>4</sub>	O <sub>2</sub>	H <sub>2</sub>
273	21	265	260	165	710	22,880	25,500	58,000
280	23	365	335	210	960	27,800	30,500	61,500
290	26	480	450	315	1300	35,200	37,600	66,500
300	30	615	570	440	1730	42,800	45,700	71,600
310	_	755	700	600	2175	50,000	52,500	76,000
320		860	835	800	2650	56,300	56,800	78,600
323		890	870	850	2870	58,000	58,000	79,000

 TABLE A.9
 Henry's Constant for Selected Gases in Water at Moderate Pressure<sup>a</sup>

<sup>a</sup>Adapted with permission from Reference 27.

501	ceteu Gases a	nu Sonus	
Gas	Solid	Т (К)	$S = C_{\Lambda,i}/p_{\Lambda,i}$ (kmol/m <sup>3</sup> ·bar)
<b>O</b> <sub>2</sub>	Rubber	298	$3.12 \times 10^{-3}$
$N_2$	Rubber	298	$1.56  imes 10^{-3}$
CO <sub>2</sub>	Rubber	298	$40.15  imes 10^{-3}$
He	SiO <sub>2</sub>	293	$0.45  imes 10^{-3}$
$H_2$	Ni	358	$9.01 \times 10^{-3}$

 TABLE A.10
 The Solubility of

 Selected Gases and Solids<sup>a</sup>

<sup>a</sup>Adapted with permission from Reference 26.

# Diffusion in a moving medium

- Examples:
  - Evaporation of water from lake under the influence of the wind or the mixing of two fluids in a pipe ]and bulk motion is caused by an external force.
- Mass diffusion in such cases is done by the mass diffusion and by the bulk motion of the medium.
- In a moving medium mass transfer is due to both diffusion and convection.



	$\bullet A \circ B$	Species	Density	Velocity	Mass flow rate
(a) Homogeneous mixture		Species A	$\rho_A = \text{constant}$	$V_A = 0$	$\dot{m}_A = 0$
(no concentration gradients	$ \circ \circ$	Species B	$\rho_B = \text{constant}$	$V_B = 0$	$\dot{m}_B = 0$
and thus no diffusion)		Mixture of A and B	$\rho = \rho_A + \rho_B$	V = 0	$\dot{m} = 0$
			= constant		
(b) Homogeneous mixture with bulk motion		Species A	$\rho_A = \text{constant}$	$V_A = V$	$\dot{m}_A = \rho_A V_A A$
(no concentration gradients	$ \circ \circ$	Species B	$\rho_B = \text{constant}$	$V_B = V$	$\dot{m}_B = \rho_B V_B A$
and thus no diffusion)		Mixture of A and B	$\rho = \rho_A + \rho_B$	V = V	$\dot{m} = \rho V A$
			= constant		$=\dot{m}_A + \dot{m}_B$
(c) Nonhomogeneous mixture without bulk motion		Species A	$\rho_A \neq \text{constant}$	$V_A = V_{{\rm diff},A}$	$\dot{m}_A = \rho_A V_{\text{diff},A} A$
(stationary medium with	$\begin{array}{c} \bullet \bullet \circ $	Species B	$\rho_B \neq \text{constant}$	$V_B = V_{{\rm diff},B}$	$\dot{m}_B = \rho_B V_{\text{diff},B} A$
concentration gradients)		Mixture of	$\rho = \rho_A + \rho_B$	V = 0	$\dot{m} = \rho V A = 0$
	$V_{\text{diff},A} \rightarrow \leftarrow V_{\text{diff},B}$	A and B	= constant		(thus $\dot{m}_A = -\dot{m}_B$ )
(d) Nonhomogeneous mixture with bulk motion		Species A	$\rho_A \neq \text{constant}$	$V_A = V + V_{{\rm diff},A}$	$\dot{m}_A = \rho_A V_{\text{diff},A} A$
(moving medium with	$ \overset{\bullet}{\bullet} \overset{\bullet}{\circ} \overset{\circ}{\bullet} \overset{\circ}{\bullet} \overset{\circ}{\circ} \overset{\circ}{\circ} \overset{\circ}{\circ} \overset{\circ}{\circ} \overset{\circ}{\circ} \overset{\circ}{\rightarrow} v $	Species B	$\rho_B \neq \text{constant}$	$V_B = V + V_{{\rm diff},B}$	$\dot{m}_B = \rho_B V_{\text{diff},B} A$
concentration gradients)	••••••	Mixture of	$\rho = \rho_A + \rho_B$	V = V	$\dot{m} = \rho V A$
	$V_{\text{diff},A} \longrightarrow \qquad \longleftarrow V_{\text{diff},B}$	A and B	= constant		$=\dot{m}_A+\dot{m}_B$


When there is no conc. gradient, no molecular mass diffusion occur in the pluid. The velocity of all species equal  $V = V_A = V_B$ 

When there is no concentration gradient, no molecular mass diffusion occur in the fluid. The velocity of all species equal to:

$$V = V_{A} = V_{B}$$

When there is concentration gradient, there will be simultaneous flow of species in the direction of decreasing concentration at a diffusion velocity of  $V_{diff}$ . The mass flow rate at any flow section is expressed as:

$$\begin{aligned} V_A &= V + V_{\text{diff},A} \\ V_B &= V + V_{\text{diff},B} \\ \dot{m}_A &= \rho_A V_A A = \rho_A (V + V_{\text{diff}}, A) A = \rho_A V A + \rho_A V_{\text{diff},A} A = \dot{m}_{\text{conv},A} + \dot{m}_{\text{diff},A} \\ \dot{m}_B &= \rho_B V_B A = \rho_B (V + V_{\text{diff},B}) A = \rho_B V A + \rho_B V_{\text{diff},B} A = \dot{m}_{\text{conv},B} + \dot{m}_{\text{diff},B} \\ j_A &= \rho_A V + \rho_A V_{\text{diff},A} = \frac{\rho_A}{\rho} \rho V - \rho D_{AB} \frac{dw_A}{dx} = w_A (j_A + j_B) - \rho D_{AB} \frac{dw_A}{dx} \\ j_B &= \rho_B V + \rho_B V_{\text{diff},B} = \frac{\rho_B}{\rho} \rho V - \rho D_{BA} \frac{dw_B}{dx} = w_B (j_A + j_B) - \rho D_{BA} \frac{dw_B}{dx} \end{aligned}$$



(a) No concentration gradient



(b) Mass concentration gradient and thus mass diffusion

$$\dot{m}_{\text{diff},A} = \rho_A V_{\text{diff},A} A = \rho_A (V_A - V) A$$
$$\dot{m}_{\text{diff},B} = \rho_B V_{\text{diff},B} A = \rho_B (V_B - V) A$$
$$\dot{m}_{\text{diff},A} + \dot{m}_{\text{diff},B} = 0 \quad \Rightarrow \quad \dot{m}_{\text{diff},A} = -\dot{m}_{\text{diff},B}$$
$$-\rho A D_{AB} \frac{dw_A}{dx} = \rho A D_{BA} \frac{dw_B}{dx}$$

Any time the species A diffuses in one direction, an equal amount of species B must diffuse in the opposite direction to maintain the density (or the molar concentration) constant.

This behavior is closely approximated by dilute gas mixtures and dilute liquid or solid solutions. For example, when a small amount of gas diffuses into a liquid, it is reasonable to assume the density of the liquid to remain constant.

$$w_A + w_B = 1$$

$$\frac{dw_A}{dx} = -\frac{dw_B}{dx}$$

 $D_{AB} = D_{BA}$ 



#### On molar basis:

$$\dot{N} = \dot{N}_A + \dot{N}_B$$

$$\rho \overline{V}A = \rho_A \overline{V}_A A + \rho_B \overline{V}_B A$$

$$\overline{V} = \frac{C_A \overline{V}_A + C_B \overline{V}_B}{C} = \frac{C_A}{C} \overline{V}_A + \frac{C_B}{C} \overline{V}_B = y_A \overline{V}_A + y_B \overline{V}_B$$

 $\overline{V}$  is called the **molar-average velocity** of the flow.

$$\dot{N}_{A} = C_{A}V_{A}A = C_{A}(\overline{V} + \overline{V}_{\text{diff},A})A = C_{A}\overline{V}A + C_{A}\overline{V}_{\text{diff},A}A = \dot{N}_{\text{conv},A} + \dot{N}_{\text{diff},A}A$$
$$\dot{N}_{B} = C_{B}V_{B}A = C_{B}(\overline{V} + \overline{V}_{\text{diff},B})A = C_{B}\overline{V}A + C_{B}\overline{V}_{\text{diff},B}A = \dot{N}_{\text{conv},B} + \dot{N}_{\text{diff},B}A$$

$$\bar{j}_A = C_A \overline{V} + C_A \overline{V}_{\text{diff},A} = \frac{C_A}{C} C \overline{V} - C D_{AB} \frac{dy_A}{dx} = y_A (\bar{j}_A + \bar{j}_B) - C D_{AB} \frac{dy_A}{dx}$$

$$\bar{j}_B = C_B \overline{V} + C_B \overline{V}_{\text{diff},B} = \frac{C_B}{C} C \overline{V} - C D_{BA} \frac{dy_B}{dx} = y_B (\bar{j}_A + \bar{j}_B) - C D_{BA} \frac{dy_B}{dx}$$

$$\dot{N}_{\text{diff},A} = C_A \overline{V}_{\text{diff},A} A = C_A (V_A - \overline{V}) A$$
$$\dot{N}_{\text{diff},B} = C_B \overline{V}_{\text{diff},B} A = C_B (V_B - \overline{V}) A$$

 $\dot{N}_{\text{diff},A} + \dot{N}_{\text{diff},B} = 0 \rightarrow \dot{N}_{\text{diff},A} = -\dot{N}_{\text{diff},B}$ 

The rates of diffusion of species *A* and *B* must be equal in magnitude but opposite in sign.

## Mass Convection

## Convective Mass Transfer

- Now we consider *mass convection* (or *convective mass transfer*), which is the transfer of mass between a surface and a moving fluid due to both *mass diffusion* and *bulk fluid motion*.
- Mass convection is usually analyzed on a *mass basis* rather than on a molar basis.

$$\frac{\rho_{A,s} - \rho_A}{\rho_{A,s} - \rho_{A,\infty}} = 0.99$$

#### Concentration boundary layer:

In mass convection, the region of the fluid in which concentration gradients exist.



Development of concentration boundary layer for species A during external flow on a flat surface.

In internal flow, we have a concentration entrance region where the concentration profile develops, in addition to the hydrodynamic and thermal entry regions.

The concentration boundary layer continues to develop in the flow direction until its thickness reaches the tube center and the boundary layers merge.

The distance from the tube inlet to the location where this merging occurs is called the concentration entry length  $L_c$ , and the region beyond that point is called the fully developed region.

$$\frac{\partial}{\partial x} \left( \frac{\rho_{A,s} - \rho_A}{\rho_{A,s} - \rho_{A,b}} \right) = 0$$
$$\rho_{A,b} = \frac{1}{A_c V_{\text{avg}}} \int_{A_c} \rho_A u dA_c$$

Prandtl number:

Schmidt number:



#### **FIGURE 14–39**

The development of the velocity, thermal, and concentration boundary layers in internal flow.

$$Pr = \frac{\nu}{\alpha} = \frac{Momentum diffusivity}{Thermal diffusivity}$$
$$Sc = \frac{\nu}{D_{AB}} = \frac{Momentum diffusivity}{Mass diffusivity}$$

Heat transfer: 
$$Pr = \frac{V}{\alpha}$$
  
Mass transfer:  $Sc = \frac{V}{D_{AB}}$ 

In mass transfer, the Schmidt plays the role of the Prandtl number in heat transfer.



A Schmidt number of near unity (Sc = 1) indicates that momentum and mass transfer by diffusion are comparable, and velocity and concentration boundary layers almost coincide with each other.

#### Ernst Heinrich Wilhelm Schmidt

(1892–1975), a German engineer, was born at Vögelsen, Germany. One of his early research efforts was a careful measurement of the radiation properties of solids, which caused him to propose and develop the use of aluminum foil as an effective radiation shield. He was the first to measure the velocity and temperature field in a free convection boundary layer and the large heat-transfer coefficients occurring in droplet condensation. The dimensionless Schmidt number which characterizes fluid flows in which there are simultaneous momentum and mass diffusion convection processes was named after him.

#### Lewis number:

 $Le = \frac{Sc}{Pr} = \frac{\alpha}{D_{AB}} = \frac{\text{Thermal diffusivity}}{\text{Mass diffusivity}}$ 



Lewis number is a measure of heat diffusion relative to mass diffusion.

#### Warren Kendall Lewis (1882–1975),

an American chemical engineer, was born in Laurel, Delaware. He was an MIT professor and through coordination of chemistry, physics, and engineering into an independent discipline to serve the chemical industry, has been called the father of modern chemical engineering. The dimensionless **Lewis number** which characterizes fluid flows in which there are simultaneous heat and mass diffusion convection processes was named after him.



$$j_{A} = \dot{m}_{A}/A_{s} = -\rho D_{AB} \frac{\partial w_{A}}{\partial y}\Big|_{y=0} \qquad (\text{kg/s} \cdot \text{m}^{2})$$
$$\dot{m}_{\text{conv}} = h_{\text{mass}}A_{s}(\rho_{A,s} - \rho_{A,\infty}) = h_{\text{mass}}\rho A_{s}(w_{A,s} - w_{A,\infty}) \qquad (\text{kg/s}) \qquad \text{rate of mass convection}$$

where  $h_{\text{mass}}$  is the average **mass transfer coefficient**, in m/s;  $A_s$  is the surface area;  $\rho_{A,s} - \rho_{A,\infty}$  is the mass concentration difference of species A across the concentration boundary layer; and  $\rho$  is the average density of the fluid in the boundary layer. The product  $h_{\text{mass}}\rho$ , whose unit is kg/m<sup>2</sup>·s, is called the *mass transfer conductance*. For internal flow we have

$$\dot{m}_{\rm conv} = h_{\rm mass} A_s \frac{\Delta \rho_{A,e} - \Delta \rho_{A,i}}{\ln \left( \Delta \rho_{A,e} / \Delta \rho_{A,i} \right)}$$

$$\Delta \rho_{A, e} = \rho_{A, s} - \rho_{A, e} \text{ and } \Delta \rho_{A, i} = \rho_{A, s} - \rho_{A, i}.$$

$$h_{\text{mass, avg}} = \frac{1}{A_s} \int_{A_s} h_{\text{mass}} dA_s \qquad \begin{array}{l} \text{average mass} \\ \text{transfer coefficient} \end{array}$$



Mass transfer at a surface occurs by diffusion because of the no-slip boundary condition, just like heat transfer occurring by conduction. Nusselt number:

$$Nu = \frac{h_{conv} L_c}{k}$$

 $Sh = \frac{h_{mass}L_c}{L_c}$ 

Sherwood number:

 $h_{\rm mass}$  is the mass transfer coefficient  $D_{AB}$  is the mass diffusivity.

The Nusselt and Sherwood numbers represent the effectiveness of heat and mass convection at the surface, respectively.

Heat transfer Stanton number:

$$\operatorname{St} = \frac{h_{\operatorname{conv}}}{\rho V c_p} = \operatorname{Nu} \frac{1}{\operatorname{Re} \operatorname{Pr}}$$

Mass transfer Stanton number:

$$\operatorname{St}_{\operatorname{mass}} = \frac{h_{\operatorname{mass}}}{V} = \operatorname{Sh} \frac{1}{\operatorname{Re} \operatorname{Sc}}$$

The Sherwood number can be obtained from the Nusselt number expression by simply replacing the Prandtl number by the Schmidt number.

$$Gr = \frac{g(\rho_{\infty} - \rho_s) L_c^3}{\rho \nu^2} = \frac{g(\Delta \rho / \rho) L_c^3}{\nu^2}$$
For natural convection mass transfer
$$Sh = f(Gr, Sc)$$

Heat transfer: 
$$Nu = \frac{h_{conv}L_c}{k}$$
  
Mass transfer:  $Sh = \frac{h_{mass}L_c}{D_{AB}}$ 

#### FIGURE 14-46

In mass transfer, the Sherwood number plays the role the Nusselt number plays in heat transfer. Analogy between the quantities that appear in the formulation and solution of heat convection and mass convection

Heat	Mass
Convection	Convection
Т	<i>С, у</i> , <i>ρ</i> , or <i>w</i>
$h_{\rm conv}$	$h_{ m mass}$
$\delta_{thermal}$	$\delta_{ ext{concentration}}$
$\operatorname{Re} = \frac{VL_{c}}{v}$	${\sf Re}=rac{VL_{ m c}}{ u}$
$\operatorname{Gr} = \frac{g\beta(T_s - T_{\infty}) L}{\nu^2}$	$\int_{-\frac{1}{c}}^{\frac{3}{c}} \operatorname{Gr} = \frac{g(\rho_{\infty} - \rho_s) L_c^3}{\rho \nu^2}$
$\Pr = \frac{\nu}{\alpha}$	$Sc = rac{ u}{D_{AB}}$
$St = \frac{h_{\mathrm{conv}}}{\rho V c_p}$	$St_{mass} = \frac{h_{mass}}{V}$
$Nu = \frac{h_{conv} L_{c}}{k}$	$Sh = \frac{h_{mass} L_{c}}{D_{AB}}$
Nu = f(Re, Pr)	Sh = f(Re, Sc)
Nu = f(Gr, Pr)	Sh = f(Gr, Sc)

Sh = f(Gr, Sc)

$$\operatorname{Gr} = \frac{g(\rho_{\infty} - \rho_s) L_c^3}{\rho \nu^2} = \frac{g(\Delta \rho / \rho) L_c^3}{\nu^2}$$

Natural convection mass transfer

Aapplicable to both temperature- and/or concentration-driven natural convection flows.

20°C		Fresh water
No convection currents		Solar pond
70°C	$\rho_{\rm brine} > \rho_{\rm water}$	Brine
Salt		

A hot fluid at the bottom will rise and initiate natural convection currents only if its density is lower.

## <u>Quiz 5</u>

- What is meaning of convective mass transfer?
- Plot the development of the velocity, thermal, and concentration boundary layers in internal flow.

#### Special Case: $Pr \approx Sc \approx 1$ (Reynolds Analogy)

$$\nu = \alpha = D_{AB} \qquad Pr = Sc = Le = 1$$

$$\frac{f}{2} Re = Nu = Sh \qquad or \qquad \frac{f}{2} \frac{VL_c}{\nu} = \frac{h_{heat}L_c}{k} = \frac{h_{mass}L_c}{D_{AB}}$$

$$\frac{f}{2} = \frac{Nu}{Re Pr} = \frac{Sh}{Re Sc} \qquad or \qquad \frac{f}{2} = St = St_{mass}$$

This relation is known as the Reynolds analogy, and it enables us to determine the seemingly unrelated friction, heat transfer, and mass transfer coefficients when only one of them is known or measured.



Reynolds analogy  $v = \alpha = D_{AB}$ (or Pr = Sc = Le)

When the molecular diffusivities of momentum, heat, and mass are equal to each other, the velocity, temperature, and concentration boundary layers coincide.

#### General Case: $Pr \neq Sc \neq 1$ (Chilton–Colburn Analogy)

0.6 < Pr < 60 and 0.6 < Sc < 3000Chilton–Colburn analogy

 $\frac{\mathrm{St}}{\mathrm{St}_{\mathrm{mass}}} = \left(\frac{\mathrm{Sc}}{\mathrm{Pr}}\right)^{2/3}$ 

 $\frac{J}{2} = \operatorname{St} \operatorname{Pr}^{2/3} = \operatorname{St}_{\text{mass}} \operatorname{Sc}^{2/3}$ 

 $\frac{h_{\text{heat}}}{h_{\text{mass}}} = \rho c_p \left(\frac{\text{Sc}}{\text{Pr}}\right)^{2/3} = \rho c_p \left(\frac{\alpha}{D_{AB}}\right)^{2/3} = \rho c_p \text{Le}^{2/3}$ 

For air–water vapor mixtures: Lewis  $h_{\text{heat}} \cong \rho c_p h_{\text{mass}}$  (air–water vapor mixtures) relation

This relation is commonly used in air-conditioning applications.

Another important consequence of  $Le \cong 1$  is that the *wet-bulb* and *adiabatic saturation temperatures* of moist air are nearly identical. In *turbulent flow*, the

Lewis relation can be used even when the Lewis number is not 1 since eddy mixing in turbulent flow overwhelms any molecular diffusion, and heat and mass are transported at the same rate. Chilton-Colburn Analogy General:  $h_{\text{mass}} = \frac{h_{\text{heat}}}{\rho c_p} \left(\frac{D_{AB}}{\alpha}\right)^{2/3}$  $= \frac{1}{2} fV \left(\frac{D_{AB}}{v}\right)^{2/3}$ Special case:  $v = \alpha = D_{AB}$  $h_{\text{mass}} = \frac{h_{\text{heat}}}{\rho c_p} = \frac{1}{2} fV$ 

When the friction or heat transfer coefficient is known, the mass transfer coefficient can be determined directly from the Chilton–Colburn analogy. Under low mass flux conditions, the mass convection coefficients can be determined by either (1) determining the friction or heat transfer coefficient and then using the Chilton–Colburn analogy or (2) picking the appropriate Nusselt number relation for the given geometry and analogous boundary conditions, replacing the Nusselt number by the Sherwood number and the Prandtl number by the Schmidt number.

Sherwood number relations in mass convection for specified concentration at the surface corresponding to the Nusselt number relations in heat convection for specified surface temperature

Convective Heat Transfer	Convective Mass Transfer
1. Forced Convection over a Flat Plate (a) Laminar flow (Re $< 5 \times 10^5$ ) Nu = 0.664 Re <sup>0.5</sup> <sub>L</sub> Pr <sup>1/3</sup> , Pr > 0.6	Sh = 0.664 $\operatorname{Re}_{L}^{0.5} \operatorname{Sc}^{1/3}$ , Sc > 0.5
(b) Turbulent flow (5 $\times$ 10 <sup>5</sup> < Re < 10 <sup>7</sup> ) Nu = 0.037 Re <sup>0.8</sup> <sub>L</sub> Pr <sup>1/3</sup> , Pr > 0.6	${\rm Sh}=0.037~{\rm Re}_{\rm L}^{0.8}~{\rm Sc}^{1/3},~{\rm Sc}>0.5$
<ul> <li>Fully Developed Flow in Smooth Circular Pipes</li> <li>(a) Laminar flow (Re &lt; 2300)</li> <li>Nu = 3.66</li> </ul>	Sh = 3.66
( <i>b</i> ) Turbulent flow (Re > 10,000) Nu = 0.023 Re <sup>0.8</sup> Pr <sup>0.4</sup> , 0.7 < Pr < 160	${\rm Sh} = 0.023 \ {\rm Re}^{0.8} \ {\rm Sc}^{0.4}, \qquad 0.7 < {\rm Sc} \ 160$
<b>3.</b> Natural Convection over Surfaces (a) Vertical plate $Nu = 0.59(Gr Pr)^{1/4}$ , $10^5 < Gr Pr < 10^9$ $Nu = 0.1(Gr Pr)^{1/3}$ , $10^9 < Gr Pr < 10^{13}$	$\begin{array}{ll} {\rm Sh}=0.59({\rm Gr}\;{\rm Sc})^{1/4}, & 10^5<{\rm Gr}\;{\rm Sc}<10^9\\ {\rm Sh}=0.1({\rm Gr}\;{\rm Sc})^{1/3}, & 10^9<{\rm Gr}\;{\rm Sc}<10^{13} \end{array}$
( <i>b</i> ) Upper surface of a horizontal plate Surface is hot $(T_s > T_\infty)$ Nu = 0.54(Gr Pr) <sup>1/4</sup> , 10 <sup>4</sup> < Gr Pr < 10 <sup>7</sup> Nu = 0.15(Gr Pr) <sup>1/3</sup> , 10 <sup>7</sup> < Gr Pr < 10 <sup>11</sup>	Fluid near the surface is light ( $\rho_s < \rho_\infty$ )Sh = 0.54(Gr Sc)^{1/4}, $10^4 < Gr Sc < 10^7$ Sh = 0.15(Gr Sc)^{1/3}, $10^7 < Gr Sc < 10^{11}$
(c) Lower surface of a horizontal plate Surface is hot ( $T_s > T_\infty$ ) Nu = 0.27(Gr Pr) <sup>1/4</sup> , 10 <sup>5</sup> < Gr Pr < 10 <sup>11</sup>	Fluid near the surface is light ( $ ho_s <  ho_\infty$ ) Sh = 0.27(Gr Sc) <sup>1/4</sup> , 10 <sup>5</sup> < Gr Sc < 10 <sup>11</sup>

#### Mass Convection Relations

## Solved Problem

 Consider a circular pipe of inner diameter D=0.015 m whose inner surface covered with a layer of liquid water as a result of condensation. In order to dry the pipe, air at 300K and 1 atm is forced to flow through it with an average velocity of 1.2 m/s. Using the analogy between heat and mass transfer, determine the mass transfer coefficient inside the pipe for developed flow.

## Solved problem

- Heat transfer coefficient in a complex geometry with complicated boundary conditions can be determined by mass transfer measurements on similar geometries under similar flow conditions using volatile solids such as naphthalene and dichlorobenzene and utilizing Chilton-Colburn analogy between heat and mass transfer at low flux condition. The amount of mass transfer during a specified time period is determined by weighing the model or measuring the surface recission.
- During the experiment involving the flow of dry air at 25 oC and 1 atm at a free stream velocity of 2m/s over a body covered with a layer naphthalene, it observed that that 12 g of naphthalene has sublimated in 15 minute. The surface area of the body is 0.3 m2. both air and the body were ket at 25 oC during the study. The vapor pressure of naphthalene at 25 oC is 11 pa and the mass diffusivity of naphthalene in air at 25 oC is DAB =0.61\*10-5 m2/s. Determine the heat transfer coefficient under the same flow condition over the same geometry.

#### Limitation on the Heat–Mass Convection Analogy

The Nusselt numbers are usually evaluated for smooth surfaces, but many mass transfer problems involve wavy or roughened surfaces.

Many Nusselt relations are obtained for constant surface temperature situations, but the concentration may not be constant over the entire surface because of the possible surface dry out.

The blowing or suction at the surface during mass transfer may also cause some deviation, especially during high speed blowing or suction.

The heat–mass convection analogy is valid for low mass flux cases in which the flow rate of species undergoing mass flow is low relative to the total flow rate of the liquid or gas mixture so that the mass transfer between the fluid and the surface does not affect the *flow velocity*.

Therefore, the heat–mass convection analogy is not applicable when the rate of mass transfer of a species is high relative to the flow rate of that species. The energy balance on a thin layer of liquid at the surface

 $\dot{Q}_{\text{sensible, transferred}} = \dot{Q}_{\text{latent, absorbed}}$  or  $\dot{Q} = \dot{m}_{\nu} h_{fg}$ 

 $\dot{m}_{\nu}$  is the rate of evaporation

 $h_{fg}$  is the latent heat of vaporization

#### **TABLE 14-14**

Various expressions for evaporation rate of a liquid into a gas through an interface area  $A_s$  under various approximations (subscript  $\nu$  stands for vapor, *s* for liquid–gas interface, and  $\infty$  away from surface)

Assumption	Evaporation Rate
General	$\dot{m}_{\nu} = h_{\rm mass} A_s (\rho_{\nu, s} - \rho_{\nu, \infty})$
Assuming vapor to be an ideal gas, $P_{\nu} = \rho_{\nu}R_{\nu}T$	$\dot{m}_{\nu} = \frac{h_{\text{mass}} A_{s}}{R_{\nu}} \left( \frac{P_{\nu, s}}{T_{s}} - \frac{P_{\nu, \infty}}{T_{\infty}} \right)$
Using Chilton–Colburn analogy, $h_{\text{heat}} = \rho c_p h_{\text{mass}} \text{Le}^{2/3}$	$\dot{m}_{\nu} = \frac{h_{\text{mass}} A_s}{\rho c_p \text{Le}^{2/3} R_{\nu}} \left( \frac{P_{\nu, s}}{T_s} - \frac{P_{\nu, \infty}}{T_{\infty}} \right)$
Using $\frac{1}{T_s} - \frac{1}{T_{\infty}} \approx \frac{1}{T}$ , where $T = \frac{T_s + T_{\infty}}{2}$	$\dot{m}_{\nu} = \frac{h_{\text{mass}} A_s}{\rho c_{\rho} \text{Le}^{2/3}} \frac{M_{\nu}}{M} \frac{P_{\nu, s} - P_{\nu, \infty}}{P}$



#### **FIGURE 14–55**

Various mechanisms of heat transfer involved during the evaporation of water from the surface of a lake.

The mixture properties such as the specific heat  $c_p$  and molar mass *M* should normally be evaluated at the *mean film composition* and *mean film temperature*. If heat transfer from the water body to the surface as well as radiation from the surroundings is negligible, which is often the case, then the heat loss by evaporation must equal heat gain by convection.

$$\dot{Q}_{\text{conv}} = \dot{m}_{\nu} h_{fg}$$
 or  $h_{\text{conv}} A_s (T_{\infty} - T_s) = \frac{h_{\text{conv}} A_s h_{fg}}{c_p \operatorname{Le}^{2/3}} \frac{M_{\nu}}{M} \frac{P_{\nu,s} - P_{\nu,\infty}}{P}$ 

Canceling  $h_{conv}A_s$  from both sides of the second equation gives

$$T_s = T_{\infty} - \frac{h_{fg}}{c_p \operatorname{Le}^{2/3}} \frac{M_{\nu}}{M} \frac{P_{\nu,s} - P_{\nu,\infty}}{P}$$

relation for the temperature of the liquid under steady conditions

## Mass Transfer coefficient for flat plates

• Several investigators have measured the evaporation from a free liquid surface-or the sublimation from a flat solid surface-of length *L* into a controlled air stream under both laminar and turbulent conditions.

$$Sh_L = 0.664 \operatorname{Re}_L^{0.5} \operatorname{Sc}^{1/3}$$
 (laminar)  $\operatorname{Re}_L < 3 \times 10^5$   
 $Sh_L = 0.036 \operatorname{Re}_L^{0.8} \operatorname{Sc}^{1/3}$  (turbulent)  $\operatorname{Re}_L \ge 3 \times 10^5$ 

• where the characteristic length in Re, and Sh, is *L*. These equations may be used if the Schmidt number is in the range 0.6 < Sc < 2500.

$$j_D = 0.664 \,\mathrm{Re}_L^{-1/2}$$
 (laminar)  $\mathrm{Re}_L < 3 \times 10^5$   
 $j_D = 0.036 \,\mathrm{Re}_L^{-0.2}$  (turbulent)  $\mathrm{Re}_L \ge 3 \times 10^5$ 

## 10atalytic Surface Reaction

-200

50

Lecture 5

### Catalytic Surface Reactions

 Such a reaction occurs at the surface of a material, can be viewed as a surface phenomenon, and can be treated as a boundary condition. Often a one-dimensional diffusion analysis may be used to approximate the performance of a catalytic reactor

 $N_{\mathrm{A},x}''(0) = \dot{N}_{\mathrm{A}}''$ 

It is also assumed that species A leaves the surface as a result of one-dimensional transfer through a thin film of thickness L and that no reactions occur within the film itself. The mole fraction of A at x = L,  $x_{A,L}$ , corresponds to conditions in the mainstream of the mixture and is presumed to be known. Representing the remaining species of the mixture as a single species B and assuming the medium to be stationary

$$\frac{d}{dx}\left(CD_{\rm AB}\frac{dx_{\rm A}}{dx}\right) = 0$$

where  $D_{AB}$  is the binary diffusion coefficient for A in B and B may be a multicomponent mixture.



## Catalytic Surface Reactions

$$\frac{d}{dx}\left(CD_{\rm AB}\frac{dx_{\rm A}}{dx}\right) = 0$$

Assuming C and DAB to be constant, Equation above may be solved subject to the conditions that

$$x_{A}(L) = x_{A,L}$$
  $N_{A,x}''(0) = -CD_{AB} \frac{dx_{A}}{dx}\Big|_{x=0} = \dot{N}_{A}''$ 

For a catalytic surface, the surface reaction rate generally depends on the surface concentration  $C_A(0)$ . For a first-order reaction that results in species consumption at the surface, the reaction rate is of the form:

 $\dot{N}_{\rm A}'' = -k_1''C_{\rm A}(0)$ 

where  $k_1''(m/s)$  is the reaction rate constant. Accordingly, the surface boundary condition, Equation above, reduces to

$$-D_{AB}\frac{dx_A}{dx}\Big|_{x=0} = -k_1''x_A(0)$$

Solving Equation above subject to the above conditions, it is readily verified that the concentration distribution is linear and of the form

$$\frac{x_{\rm A}(x)}{x_{\rm A,L}} = \frac{1 + (xk_1''/D_{\rm AB})}{1 + (Lk_1''/D_{\rm AB})}$$

At the catalytic surface this result reduces to

$$\frac{x_{\rm A}(0)}{x_{\rm A,L}} = \frac{1}{1 + (Lk_1''/D_{\rm AB})}$$

## Catalytic Surface Reactions....

• The Molar flux is :



• The negative sign implies mass transfer to the surface

## Two limiting cases

- . For the limit  $k_1^{\prime\prime} o 0$
- For the limit  $k_1'' \rightarrow 0$ ,  $(Lk_1''/D_{AB}) << 1$  and Equations reduce to

 $\frac{x_{\mathrm{A},s}}{x_{\mathrm{A},L}} \approx 1$  and  $N''_{\mathrm{A}}(0) \approx -k''_{\mathrm{I}}Cx_{\mathrm{A},L}$ 

 In such cases the rate of reaction is controlled by the reaction rate constant, and the limitation due to diffusion is negligible. The process is said to be reaction limited. For the limit  $k_1'' \to \infty$ •  $(Lk_1''/D_{AB}) >> 1$  $x_{A,s} \approx 0$  and  $N_A''(0) \approx -\frac{CD_{AB}x_{A,L}}{L}$ 

In this case the reaction is controlled by the rate of diffusion to the surface, and the process is said to be diffusion limited

## Mass Diffusion with Homogeneous Chemical Reactions

Lecture 6

# Mass Diffusion with Homogeneous Chemical Reactions

• If we also assume steady, one-dimensional transfer in the *x*-direction and that  $D_{AB}$  and *C* are constant, Equation reduces to

$$D_{\rm AB}\frac{d^2C_{\rm A}}{dx^2} + \dot{N}_{\rm A} = 0$$

• The volumetric production rate,  $\dot{N}_A$ , is often described using one of the following forms.

Zero-Order Reaction 
$$\dot{N}_{A} = k_{0}$$

 $N_{\rm A} = k_1 C_{\rm A}$ 

First-Order Reaction

Conditions must be applied to mass transfer with Homogenous Chemical reaction...

• If  $\dot{N}_A$  is positive, the reaction results in the generation of species A

• if  $\dot{N}_A$  is negative, it results in the consumption of A

## First Order Chemical Reaction

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$$D_{\rm AB}\frac{d^2C_{\rm A}}{dx^2} - k_1C_{\rm A} = 0$$

• The linear homogenous differential equation has the general solution

$$C_A(x) = C_1 e^{mx} + C_2 e^{-mx}$$

where m  $(k_1/D_{AB})^{1/2}$  and the constants  $C_1$  and  $C_2$  depend on the prescribed boundary conditions.

## Boundary Conditions

• Gas A is soluble in liquid B, where it is transferred by diffusion and experiences a first-order chemical reaction. The solution is dilute, and the concentration of A in the liquid at the interface is a known constant CA,0. If the bottom of the container is impermeable to A, the boundary conditions are

 $C_{\rm A}(0) = C_{\rm A,0}$  and  $\frac{dC_{\rm A}}{dx}\Big|_{x=L} = 0$ 

$$C_{\rm A}(x) = C_{{\rm A},0} \frac{\cosh m(L-x)}{\cosh mL}$$



Quantities of special interest are the concentration of A at the bottom and the flux of A across the gas-liquid interface.



### Moreover,

$$N_{A,x}''(0) = -D_{AB} \frac{dC_A}{dx} \bigg|_{x=0}$$
$$= D_{AB} C_{A,0} m \frac{\sinh m(L-x)}{\cosh mL} \bigg|_{x=0}$$

 $N_{A,x}''(0) = D_{AB}C_{A,0} m \tanh mL$ 

## Solved Problem

• Biofilms, which are colonies of bacteria that can cling to living or inert surfaces, can cause a wide array of human infections. Infections caused by bacteria living within biofilms are often chronic because antibiotics that are applied to the surface of a biofilm have difficulty penetrating through the film thickness. Consider a biofilm that is associated with a skin infection. An antibiotic (species A) is applied to the top layer of a biofilm (species B) so that a fixed concentration of medication,  $C_{A,0} = 4 \times 10^{-3} \text{ kmol/m}^3$ , exists at the upper surface of the biofilm. The diffusion coefficient of the medication within the biofilm is  $D_{AB} = 2 \times 10^{-12} \text{ m}^2/\text{s}$ . The antibiotic is consumed by biochemical reactions within the film, and the consumption rate depends on the local concentration of medication expressed as  $N_A = k_1 C_A$  where  $k_1$ =0.1 s<sup>-1</sup>. To eradicate the bacteria, the antibiotic must be consumed at a rate of at least 0.2  $\times$  10<sup>-3</sup> kmol/s m<sup>3</sup> ( $\dot{N}_A \leq -0.2 \times 10^{-3}$  kmol/s m<sup>3</sup>) since, at smaller absolute consumption rates, the bacteria will be able to grow back faster than it is destroyed. Determine the maximum thickness of a biofilm, L, that may be treated successfully by the antibiotic?.

