

# TRANSPORT 1

CHEM 0915341

Summer Semester 21/22

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## CHAPTER 2

## MOLECULAR TRANSPORT MECHANISM



## GENERAL OBJECTIVE

- To be able to understand and relate the fundamental mechanisms of **mass, heat, and momentum transport** at the **molecular and turbulent regime** that would cover:
  1. Evaluation of **transport properties correlations**;
  2. Use of transport principles to **interphase transfer**;
  3. **Integration of rate equations** for systems with variable concentration along the length of contacting path; and
  4. Integration of transport phenomena to **industrial equipment design**.



# **PART ONE**

- **Introduction to Transport Phenomena**
- **Molecular Transport Mechanism**
  - **The General Molecular Transport Equation**
    1. **Mass Transport**
    2. **Heat Transport**
    3. **Momentum Transport**



## UNIT OPERATION & PROCESS

Q. Differentiate a chemical process from a unit operation. Give at least five examples for each.

### CHEMICAL PROCESS (Foust et. al, 1980)

“...may consist of widely varying sequence of steps, the principles of which are independent of the material being operated upon and of other characteristics of each particular system.”

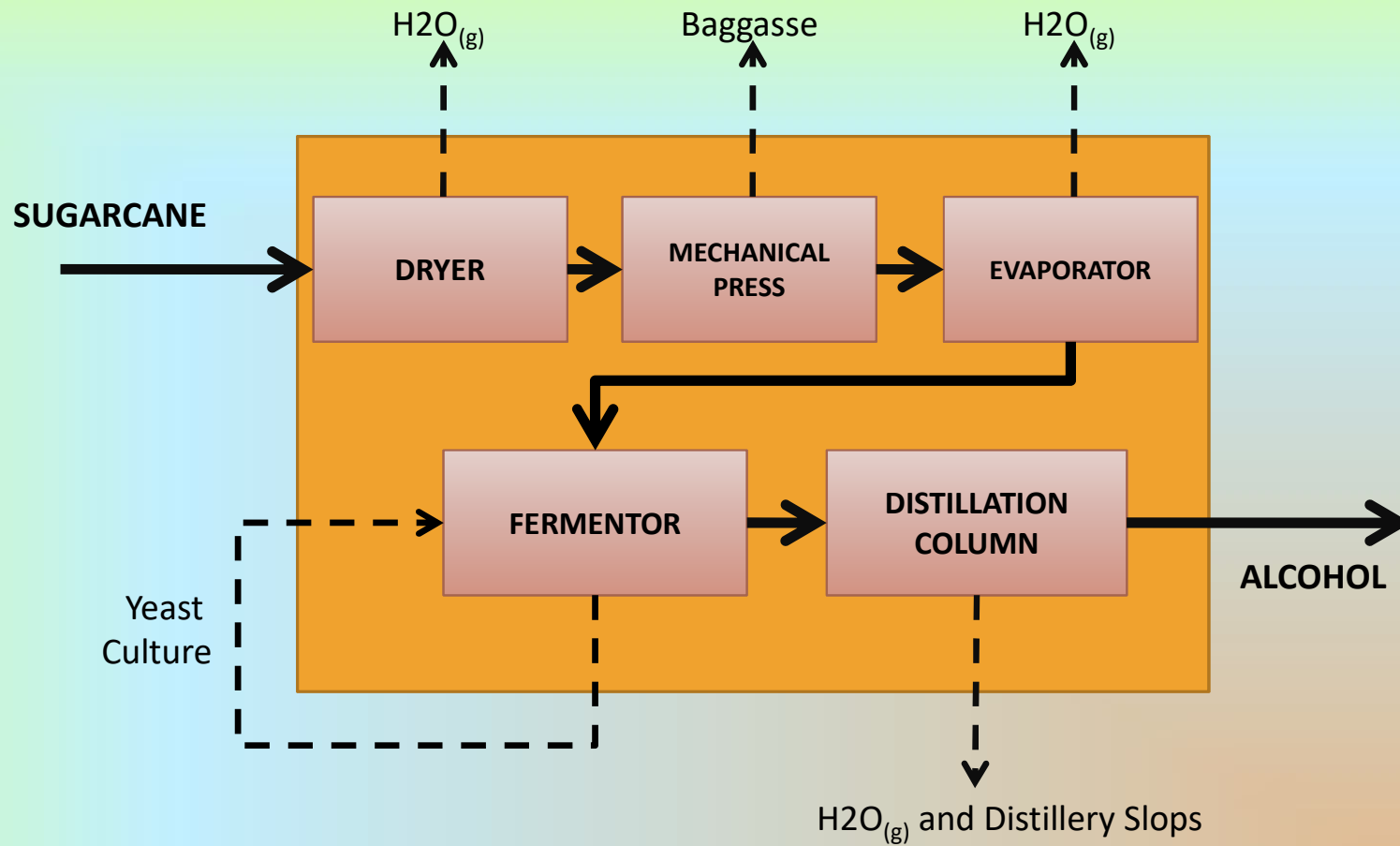
**Examples:** biodiesel production, sugar processing/refining, food processing, waste treatment

### UNIT OPERATIONS (Foust et. al, 1980)

“...individual steps that break up a complex process; which are identical in fundamentals regardless of the material being processed.”

**Examples:** pulverizing, mixing, heating, roasting, crystallization, drying, screening, electrolysis, fluid flow, distillation, humidification, gas absorption





SIMPLIFIED BLOCK DIAGRAM FOR ALCOHOL PROCESSING

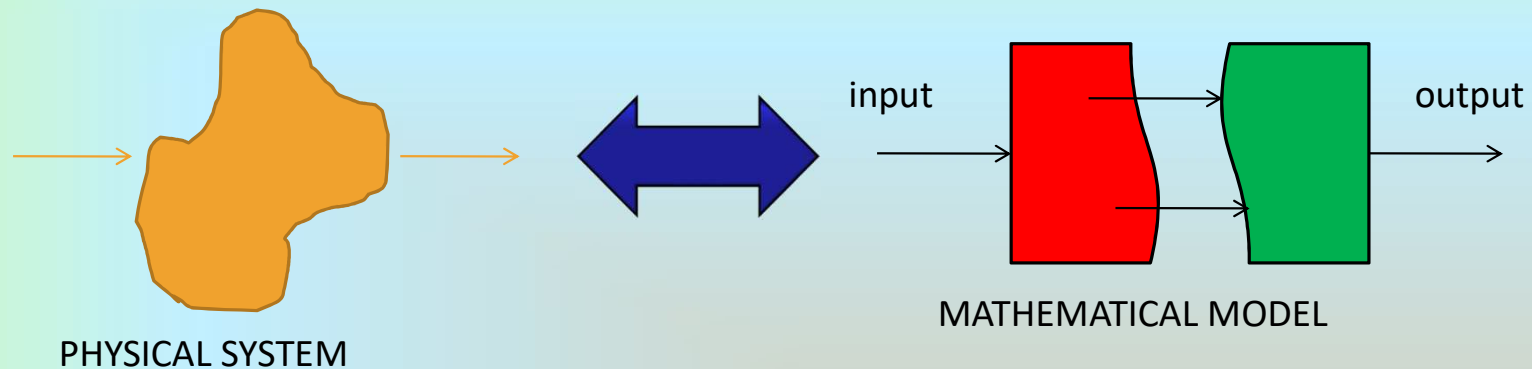


*“The complexity of chemical engineering results from the variety of conditions as to temperature, pressure, etc. under which the unit actions must be carried out in different processes along with other limitations of the operation.*

**Foust et. al, 1980**



# TRANSPORT PHENOMENA



- When chemical rates and equilibria are known, chemical changes as well as physical changes may be mathematically modeled into unit operation calculations.



## Three Major Properties Involved in Transport Phenomena



Transport Phenomena in a Heat Exchanger

**Mass** – the property of an object that is a measure of its inertia, the amount of matter it contains, and its influence in a gravitational field

**Heat** – energy perceived as temperature; a form of transferred energy (conduction, convection, radiation) that arises from the random motion of molecules

**Momentum** – measure of movement; quantity that expresses the motion of a body and its resistance to slowing down





## Three Major Properties Involved in Transport Phenomena



**Momentum Transport:** fluid flowing through the heat exchanger

**Heat Transport:** exchange of heat between the cold and the hot fluids

**Mass Transport:** presence of phase change

Note: **TRANSPORT vs TRANSFER**

Transport → refers to the fundamental mechanism in a single phase

Transfer → refers to the overall process



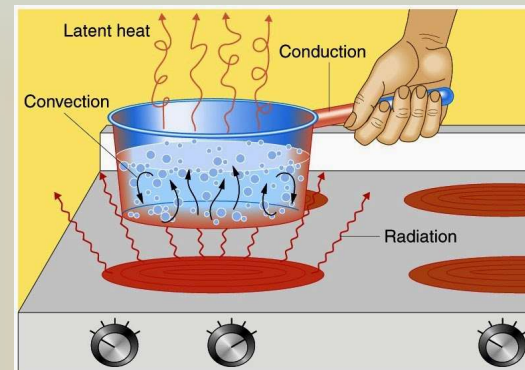
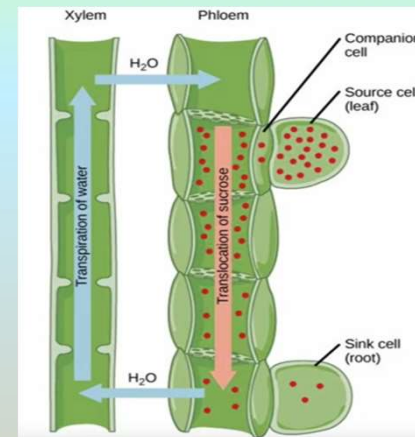
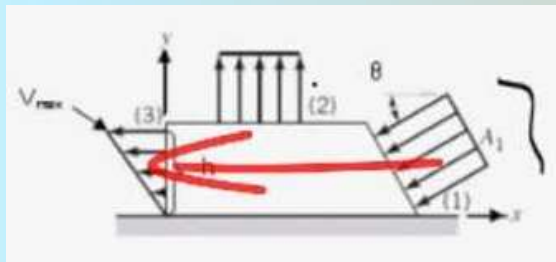
## Three Major Properties Involved in Transport Phenomena

MASS	HEAT	MOMENTUM
Leaching/Extraction Gas Absorption Distillation Humidification Crystallization	Heat exchanger	Piping system, agitation and mixing of fluids
Evaporation		
Drying of solids		



# CONCERNS IN TRANSPORT PHENOMENA

- **Mass Transport:** to describe the process
- **Energy Transport:** to predict heat exchange performance
- **Momentum Transport:** to yield prediction of pressure losses in a piping system



## TWO MECHANISMS OF TRANSPORT

### ▪ **Molecular Transport**

- ✓ Depends upon the motion of individual particles
- ✓ Transport occurring due to aggregate group of molecules

### ▪ **Turbulent/Convective Transport**

- ✓ Results from the motion of large groups or cluster of molecules



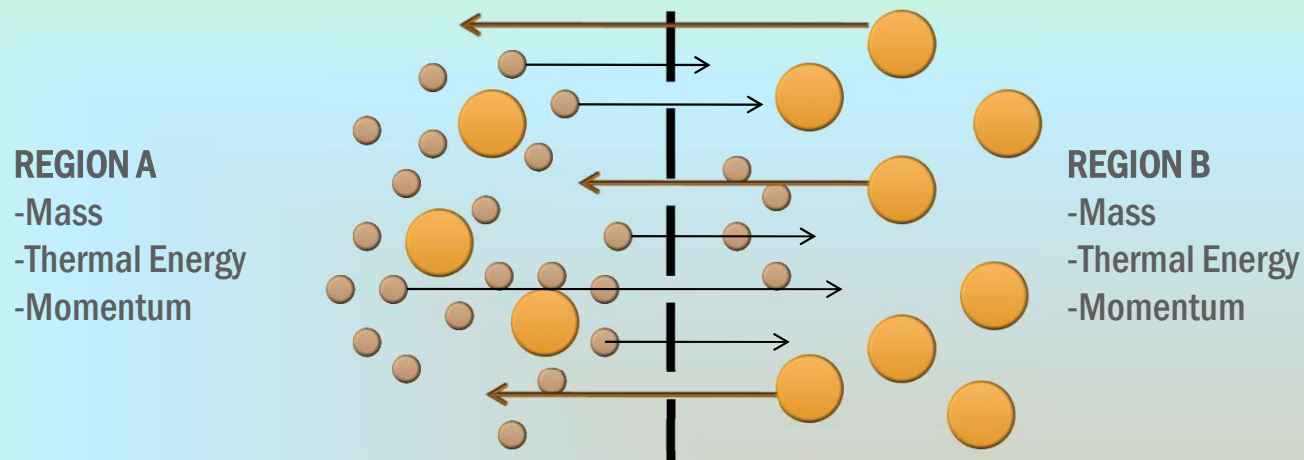
# MOLECULAR TRANSPORT MECHANISM

## Objectives:

1. To understand molecular transport mechanism from a study of the **kinetic theory of gases and liquids** or from a consideration of **solid-state physics**;
2. From a simplified physical model of a fluid, to be able to **derive an expression for the rate of transport** as a **function of a concentration gradient**, which will be extended to real gases, liquids, and solids; and
3. To **predict transport properties** of gases, liquids, and solids from a given correlation obtained from experimental data.



# Molecular Transport



Due to concentration gradient, net transport occurs.

- Transport of mass, heat, and momentum occurs among **solids, liquids, and gases**.
- Due to the substantial **differences in molecular structure**, the actual mechanism of transport differs greatly



PHYSICAL STATE	CHARACTERISTICS	IMPLICATION
<b>GAS</b>	<ul style="list-style-type: none"> <li>Few molecules per unit volume</li> <li>Intermolecular Forces of Attraction (IMFA) relatively weak</li> <li>Molecules move at random motion</li> </ul>	<ul style="list-style-type: none"> <li>Molecules move relatively freely for considerable distance before colliding</li> </ul>
<b>LIQUID</b>	<ul style="list-style-type: none"> <li>Relatively contain higher concentration of molecules per unit volume than gases</li> <li>Relatively has higher IMFA than gases</li> <li>Molecular motion is much more restricted</li> </ul>	<ul style="list-style-type: none"> <li>Migration of molecules from one region to another is at lower rate than in gases</li> </ul>
<b>SOLID</b>	<ul style="list-style-type: none"> <li>Closely-packed/highly ordered structure</li> <li>IMFA are strong enough to form crystal lattice</li> </ul>	<ul style="list-style-type: none"> <li>Freedom of movement is restricted to small vibrations in lattice sites</li> <li>Lattice molecular motion</li> </ul>



# Molecular Transport

From the three physical states, two important factors were considered:




1. **Molecular Diffusion** – the flow of energy or matter from higher concentration to a lower concentration resulting in an even distribution (equilibrium)
2. **Molecular Collision** – collision of molecules vibrating at relatively fixed conditions in conduction





# Molecular Transport

- In summary...

PHYSICAL STATE	MASS TRANSPORT (Molecular Diffusion)	HEAT TRANSPORT (Molecular Collision)	MOMENTUM TRANSPORT (Diffusion & Collision)
GASES			
LIQUIDS			
SOLIDS			



## Review

1. What are the two molecular transport mechanism?
2. What are the respective driving force/s of heat, mass and momentum transport?
3. Differentiate transport and transfer.
4. Differentiate flux and gradient.
5. Differentiate molecular diffusion and molecular collision.



## THE GENERAL MOLECULAR TRANSPORT EQUATION

- Influenced by the “simple model gas”, which was first derived by James Clerk Maxwell (1860)
  - Derived from the assumptions in the model of “ultrasimplified kinetic theory of gases” which are based on the Ideal Gas and Kinetic Theory of Gases.
- 
- **Assumptions**
    1. The gas is made up of molecules, each which is a perfect sphere,  $D = \sigma$
    2. Negligible attractive & repulsive forces between gas molecules
    3. Each molecule is in random motion at a mean speed,  $\bar{c}$ .



## Assumptions

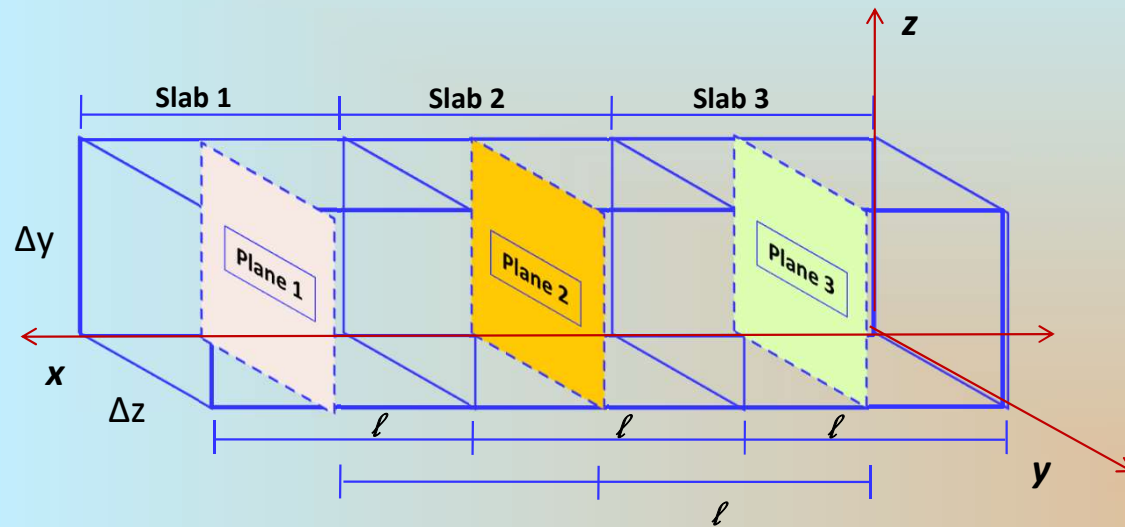
4. Actual volume of the molecules is negligible compared to the volume between molecules
5. Perfectly elastic collision between molecules
6. Each molecule moves a distance  $l$  between collisions with other molecules. The distance  $l$  is called “mean free path”.
7. The time required for a molecule to travel a mean free path travelling at the mean speed is the mean time between collisions,  $\theta$ .

$$\bar{\theta} = \frac{l}{c}$$

8. The number of molecules is large enough that statistically average values of properties can be used to describe the system.

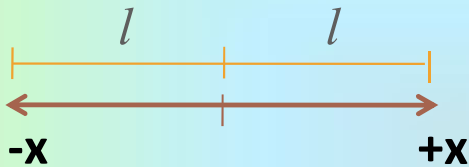


- Consider the volume element of the model gas,
- Let:
  - ✓  $\Gamma$  = transferent property; concentration of the property to be transferred
  - ✓  $(d\Gamma/dx)$  = gradient; increase in concentration at a certain distance,  $l$



## Possible Movement of Molecule in a Volume Element

### 1. One-dimensional flow



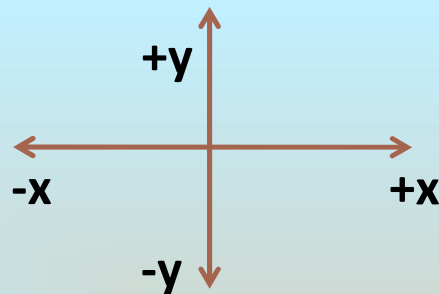
Two coordinate axes (+x, -x)

$l$  - mean free path

$\theta$  - mean time

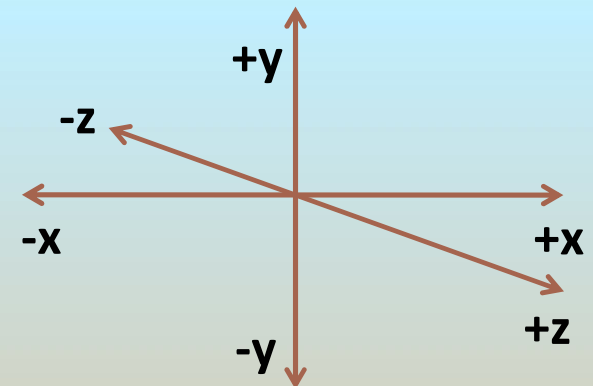
$N = c = \text{mean speed} = l/\theta$

### 2. Two-dimensional flow



Four coordinate axes  
(+x -x, +y -y)

### 3. Three-dimensional flow



Six coordinate axes  
(+x -x, +y -y, +z -z)



## DEFINITION OF TERMS (GRADIENT)

$\Gamma$  - concentration of transferent property

- amount of transferent property/volume

$P$  - amount of transferent property

$V$  - volume of the element

$\Gamma_1$  - concentration of transferent property in slab 1

$\Gamma_2$  - concentration of transferent property in slab 2

$\Gamma_3$  - concentration of transferent property in slab 3



- For the amount of gas

$$P_1 = \Gamma_1 V$$

$$P_2 = \Gamma_2 V$$

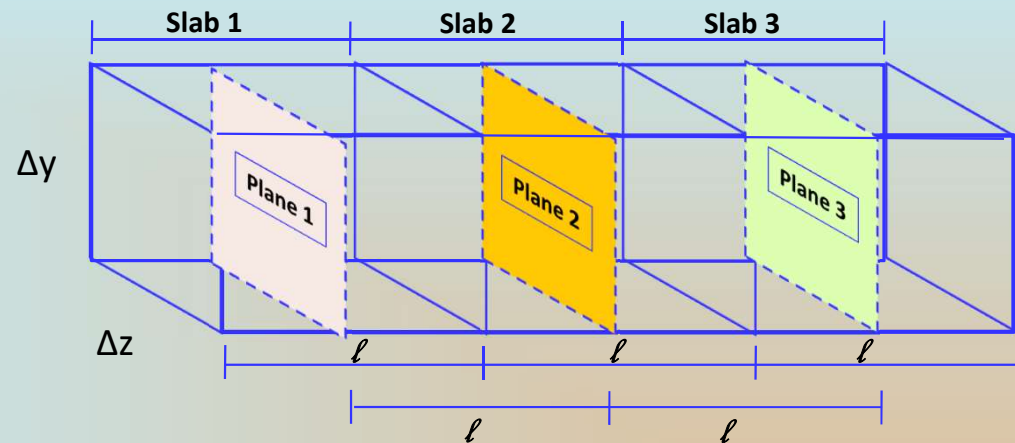
$$P_3 = \Gamma_3 V$$

But  $V = l\Delta y\Delta z$

Then  $P_1 = \Gamma_1 l\Delta y\Delta z$

$$P_2 = \Gamma_2 l\Delta y\Delta z$$

$$P_3 = \Gamma_3 l\Delta y\Delta z$$





- Consider the movement of molecule from plane to plane

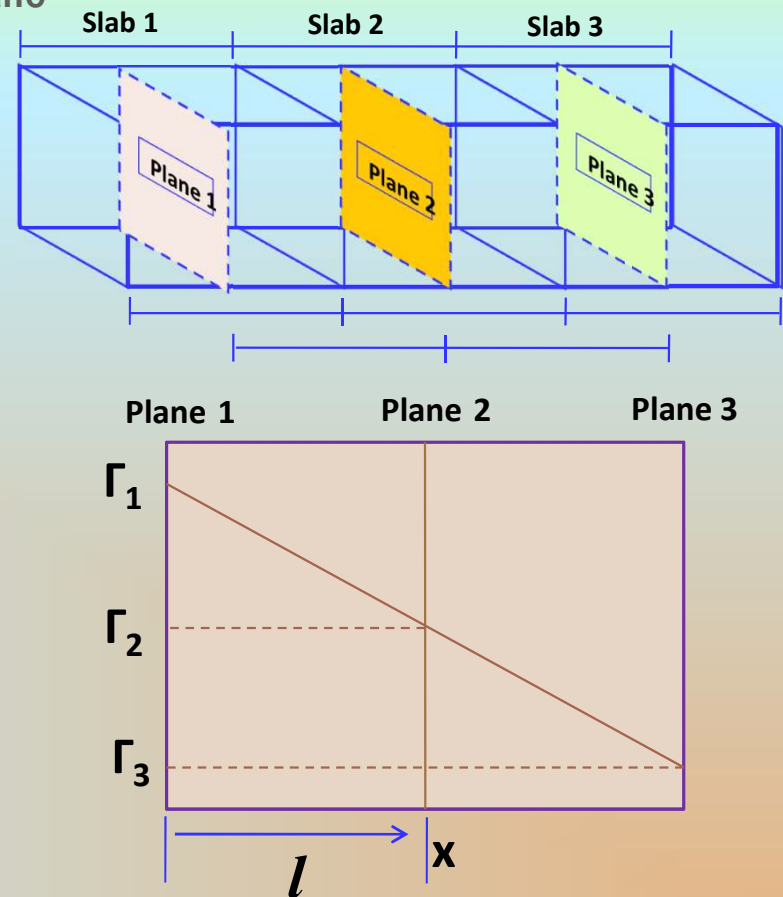
Slope:

$$-\frac{d\Gamma}{dx} = \frac{\Gamma_2 - \Gamma_1}{-l}$$

$$\Gamma_1 = \Gamma_2 - \frac{ld\Gamma}{dx}$$

$$\Gamma_2 = \Gamma_3 - \frac{ld\Gamma}{dx}$$

$$\Gamma_3 = \Gamma_2 + \frac{ld\Gamma}{dx}$$



## FLUX

$\Psi = \Phi = F$  = flux of transferent property

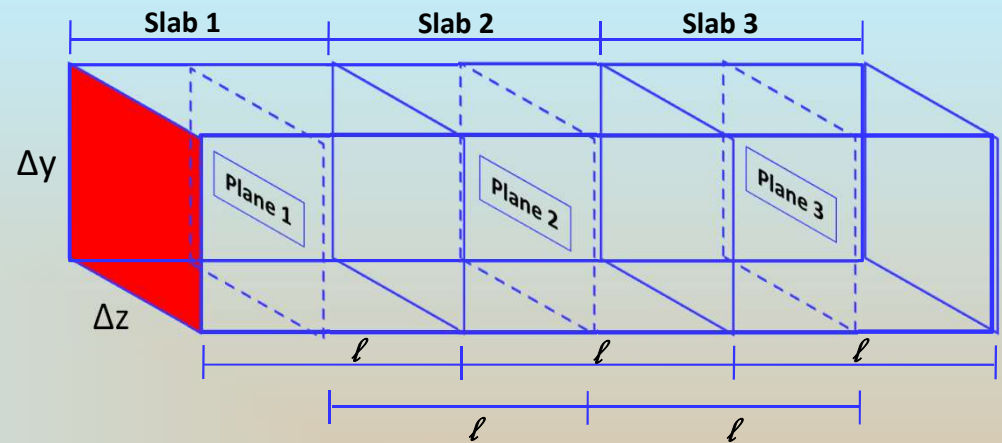
*flow of transferent/time*  
*transferent area*

$$\Psi = \frac{P/\theta}{A}$$

$$\Psi = \frac{\text{rate of transferent property}}{\text{transferent area}}$$

$$\Psi = \frac{dP/dt}{A}$$

$$A = \Delta y \Delta z$$



- Assuming that 1/6 of the total amount of the transferent property migrates along the +x axis

$$P_1 = \frac{\Gamma_1 l \Delta y \Delta z}{6} \quad P_2 = \frac{\Gamma_2 l \Delta y \Delta z}{6} \quad P_3 = \frac{\Gamma_3 l \Delta y \Delta z}{6}$$

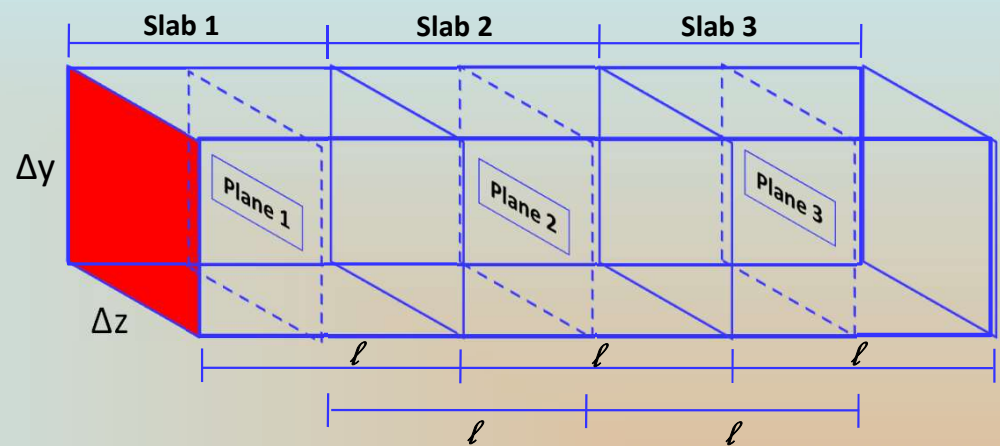
- Flux from plane 1-2:

$$\Psi_{1-2} = \frac{\Gamma_1 l \Delta y \Delta z / (6\theta)}{\Delta y \Delta z} = \frac{\Gamma_1 l}{6\theta}$$

$$\Psi_{2-1} = \frac{-\Gamma_2 l}{6\theta}$$

$$\Psi_{2-3} = \frac{\Gamma_2 l}{6\theta}$$

$$\Psi_{3-2} = \frac{-\Gamma_3 l}{6\theta}$$



- Net Flux from plane 1-2

$$\Psi_{net\ 1-2} = \Psi_{1-2} + \Psi_{2-1} = \frac{\Gamma_1 l}{6\theta} - \frac{\Gamma_2 l}{6\theta}$$

$$\Psi_{net\ 1-2} = \frac{l}{6\theta} (\Gamma_1 - \Gamma_2) = \frac{\Gamma_1 l}{6\theta} - \frac{\Gamma_2 l}{6\theta}$$

- But  $\Gamma_1 = \Gamma_2 - \frac{ld}{dx}$

$$\therefore \Psi_{net\ 1-2} = \frac{l}{6\theta} \left( \Gamma_2 - \frac{ld\Gamma}{dx} - \Gamma_2 \right)$$

$$\Psi_{net\ 1-2} = \frac{-l^2}{6\theta} \left( \frac{d\Gamma}{dx} \right)$$

- And  $c = v = \frac{l}{\theta}; \theta = \frac{l}{c}$

$$\Psi_{net\ 1-2} = \frac{-lc}{6} \left( \frac{d\Gamma}{dx} \right)$$



# The General Molecular Transport Equation

- For steady state processes,

$$\Psi = -\frac{1}{6} l \bar{c} \left( \frac{d\Gamma}{dx} \right)$$

Generalized molecular transport equation



## SEATWORK

### Derivation of the Net Flux from plane 2-3

- Net Flux from plane 2-3

$$\Psi_{net\ 2-3} = \Psi_{2-3} + \Psi_{3-2} = \frac{\Gamma_2 l}{6\theta} - \frac{\Gamma_3 l}{6\theta}$$

$$\Psi_{net\ 2-3} = \frac{l}{6\theta} (\Gamma_2 - \Gamma_3) = \frac{\Gamma_1 l}{6\theta} - \frac{\Gamma_2 l}{6\theta}$$

- But  $\Gamma_2 = \Gamma_3 - \frac{ld\Gamma}{dx}$

$$\therefore \Psi_{net\ 2-3} = \frac{l}{6\theta} \left( \Gamma_3 - \frac{ld\Gamma}{dx} - \Gamma_3 \right)$$

$$\Psi_{net\ 2-3} = \frac{-l^2}{6\theta} \left( \frac{d\Gamma}{dx} \right)$$

- And  $c = V = \frac{l}{\theta}; l = c\theta$

$$\Psi_{net\ 2-3} = \frac{-lc}{6} \left( \frac{d\Gamma}{dx} \right)$$



# Heat, Mass, and Momentum Transport

## Phenomenological Laws

- **Mathematical expressions** which describe how matter undergoes heat, mass, and momentum transport on a molecular level
- These are based on the observations of the **natural phenomena**



*“The practical applications of mass, heat, and momentum transport developed before the basic mechanisms were understood. The engineers who applied the principles of the three types of transport were not primarily interested in the similarities among the mechanisms of transport.”*

*Foust et. al, 1980*



# Heat, Mass, and Momentum Transport

## Phenomenological Laws

- **Fourier's Law of Heat Conduction** (Heat Transport)
- **Fick's Law of Molecular Diffusion** (Mass Transport)
- **Newton's Law of Viscosity** (Momentum Transport)





## Heat, Mass, and Momentum Transport

### Fourier's Law of Heat Conduction

$$Q = \frac{q}{A} = -k \frac{dT}{dx}$$

Where:	$Q$	=	heat flux (W/m <sup>2</sup> )
	$q$	=	heat transfer rate (W or J/sec)
	$A$	=	area
	$k$	=	thermal conductivity
	$\frac{dT}{dx}$	=	temperature gradient along x



## Heat, Mass, and Momentum Transport

### Fick's Law of Molecular Diffusion

$$\overline{N}_a = \frac{N_a}{A} = -D \frac{dC_a}{dx}$$

Where:

$\overline{N}_a$

=

mass flux

$N_a$

=

mass transfer rate

$A$

=

area

$D$

=

mass diffusivity

$\frac{dC_a}{dx}$

=

concentration gradient along x



## Heat, Mass, and Momentum Transport

### Newton's Law of Viscosity

$$\tau_{yx} = \frac{F_y}{A} g_c = -\mu \frac{dV_y}{dx}$$

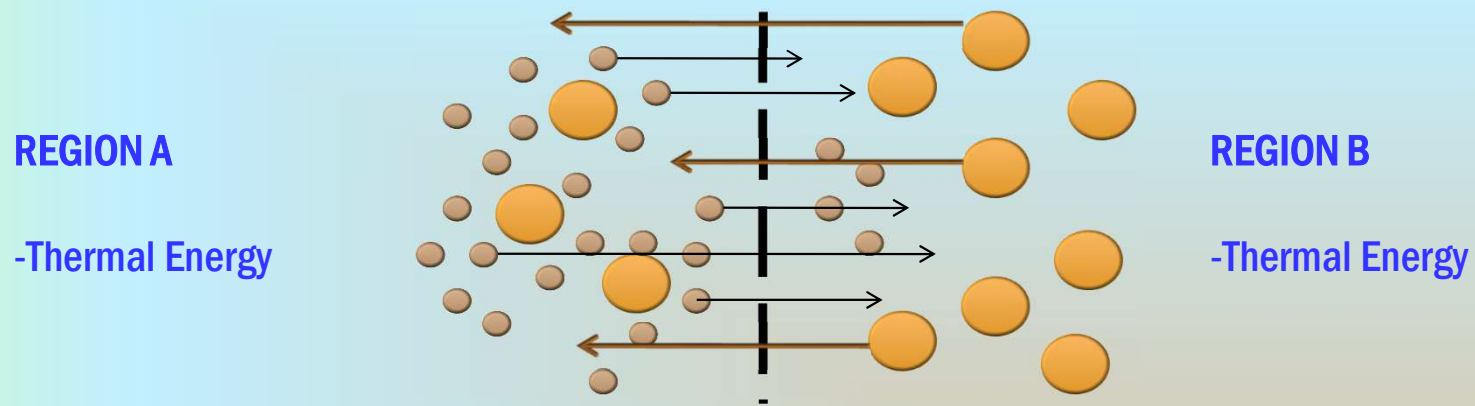
Where:

$\tau_{yx}$	=	momentum flux
y	=	direction of flow (velocity)
x	=	momentum flux
$\mu$	=	absolute viscosity
$\frac{dV_y}{dx}$	=	velocity gradient along x
$\frac{F_y}{A}$	=	shear stress
$g_c$	=	gravitational constant



## Heat, Mass, and Momentum Transport

### Heat/Thermal Energy Transport



### Generalizations:

- Temperature is conceived from the movement of the molecules
- The higher the temperature of the system, the greater is the concentration of thermal energy.



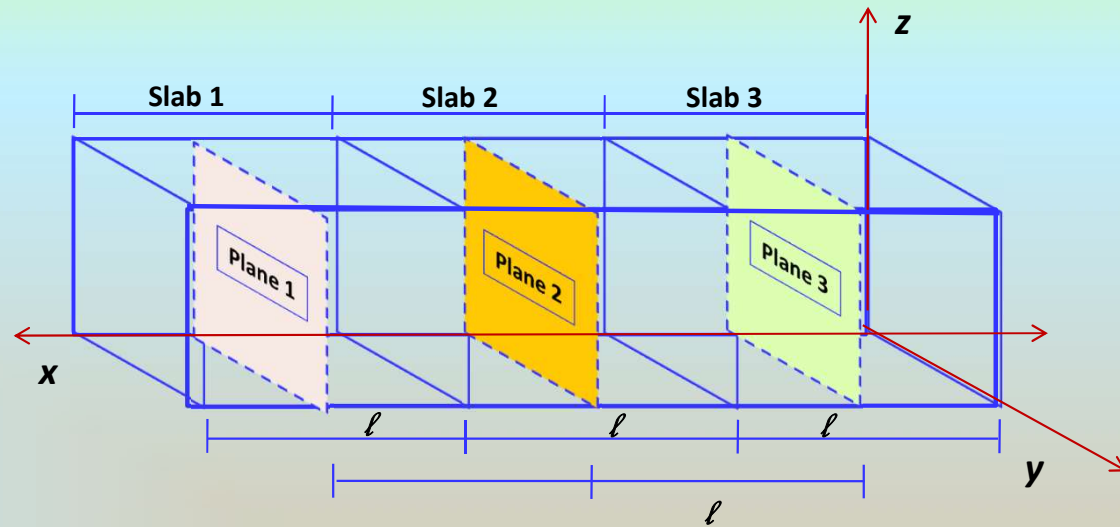
## Heat, Mass, and Momentum Transport

### Heat/Thermal Energy Transport

#### Extended Molecular Heat Transport Equation

$$Q = \frac{q}{A} = -\alpha \frac{d(\rho C_p T)}{dx} = -k \frac{dT}{dx}$$

where:  $\alpha$  = thermal diffusivity



#### Sample Problem1:

Calculate the heat flux across a copper block 10 cm thick, one side of which is maintained at 0°C and the other at 100°C. The  $k$  can be assumed constant at 380 W/m-K.



Solution:

$$\frac{q}{A} = -k \frac{dT}{dx}$$

Integration:

$$\int_{x_1}^{x_2} \left(\frac{q}{A}\right) \cdot dx = -k \int_{T_1}^{T_2} dT$$

The integration will become:

$$\left(\frac{q}{A}\right) \cdot (x_2 - x_1) = -k[T_2 - T_1]$$

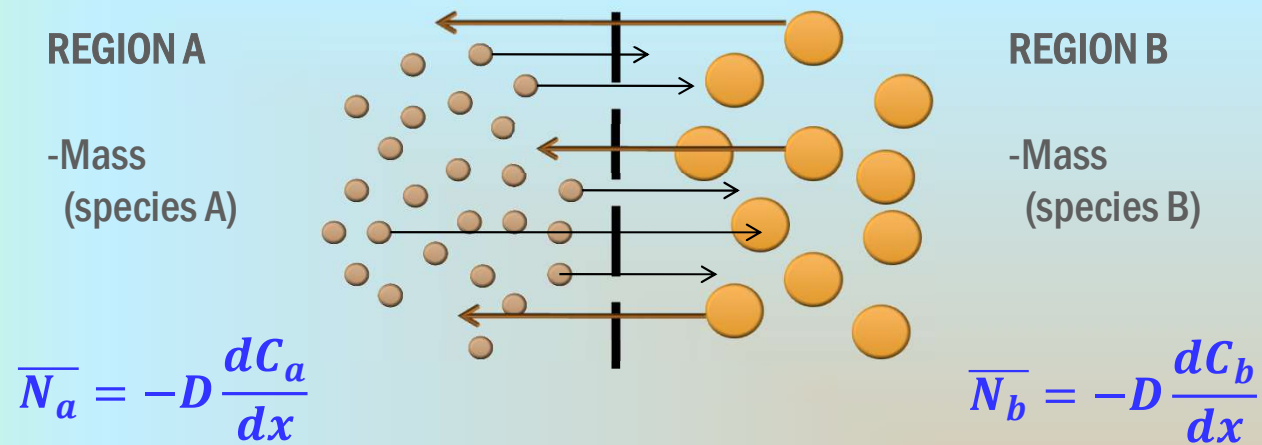
Substituting the given information:

$$\left(\frac{q}{A}\right) = -3.8 \times 10^5 J \cdot m^{-2} s^{-1}$$



## Heat, Mass, and Momentum Transport

### MASS TRANSPORT: Equimolar Counter Diffusion (ECD)



#### Generalizations:

The boundaries of the system are permeable to both components.

At constant T & P, both A and B will diffuse because of concentration gradient.



For system containing A&B species:

Assume  $C_{a1} > C_{a2} > C_{a3}$  and  $C_{b1} < C_{b2} < C_{b3}$

Gradient

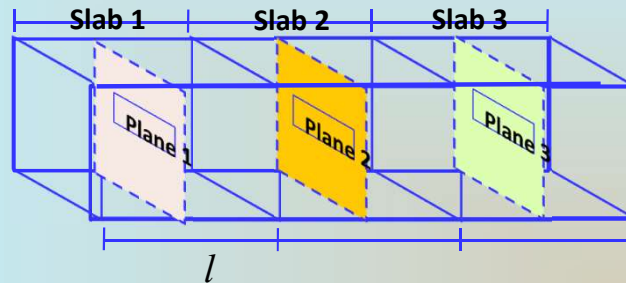
$$\frac{d\Gamma}{dx} = \frac{(\Gamma_2 - \Gamma_1)}{l}$$

$$\Gamma_1 = \Gamma_2 - \frac{ld\Gamma}{dx}$$

Flux

$$\Psi_{1-2} = \frac{\Gamma_1 l}{6\theta} \quad \text{and} \quad \Psi_{2-1} = \frac{-\Gamma_2 l}{6\theta}$$

$$\text{Then } \Psi_{net\ 1-2} = \frac{-l}{6} \left( \frac{d\Gamma}{dx} \right)$$



$$\frac{dC_a}{dx} = \frac{C_{a2} - C_{a1}}{l}$$

$$C_{a1} = C_{a2} - \frac{ldC_a}{dx}$$

Similarly

$$C_{a2} = C_{a3} - \frac{ldC_a}{dx}$$

$$\Psi_{1-2} = \frac{C_{a1} l}{6\theta}$$

$$\Psi_{2-1} = \frac{-C_{a2} l}{6\theta}$$

$$\Psi_{net\ 1-2} = \frac{-lc}{\theta} \left( \frac{dC_a}{dx} \right)$$





$N_a$   $\longrightarrow$  mass rate of component **a**

$A$   $\longrightarrow$  transfer area

$$\left(\frac{N_a}{A}\right)_{net} = \frac{-lc}{6} \frac{dC_a}{dx}$$

$\frac{lc}{6} \rightarrow D$  is mass diffusivity

$\delta$  is transport diffusivity

For substance B

$$\left(\frac{N_b}{A}\right)_{net} = \frac{-lc}{6} \frac{dC_b}{dx}$$

For ideal gas

$$D = \frac{lc}{6}$$

For real gases or liquids,

$D$  is determined experimentally

$$\left(\frac{N_a}{A}\right)_{net} = -D \frac{dC_a}{dx}$$

$$\left(\frac{N_b}{A}\right)_{net} = -D \frac{dC_b}{dx}$$

**What is the relation between these two equations?**

**These equations are Fick's Law of Diffusion**



$V_t$  - total volume of mixture/ container

$V_a$  - volume of component a

$V_b$  - volume of component b

At constant T and P, V is constant

$$V_a = V_t = V_b$$

$m_t$  - total mass of the mixture

$$m_t = m_a + m_b$$

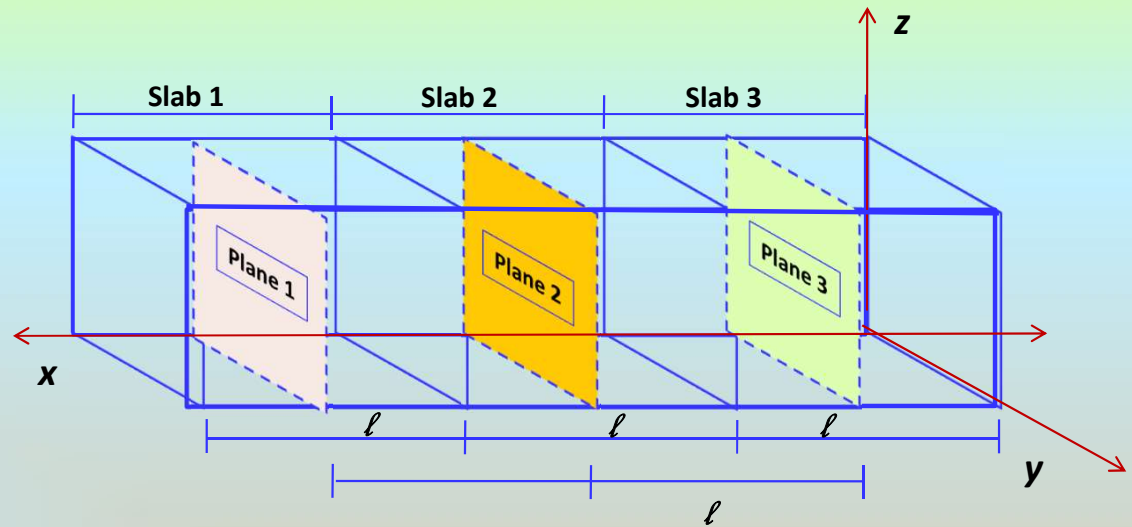
The diffusion rate of A and B are interrelated by the total concentration

$$V_t C_t = V_a C_a + V_b C_b \text{ and since } V \text{ is constant, then } C_t = C_a + C_b$$

Differentiate the last equation with respect to x:

$$0 = \frac{dC_a}{dx} + \frac{dC_b}{dx} \text{ and } \frac{dC_a}{dx} = -\frac{dC_b}{dx} \quad (1)$$

The gradient of B is equal to but opposite sign to that of gas A.



$$\left(\frac{N_a}{A}\right)_{net} = -D \frac{dC_a}{dx}$$

$$\frac{dC_a}{dx} = -\frac{\left(\frac{N_a}{A}\right)_{net}}{D} \quad (2)$$

$$\left(\frac{N_b}{A}\right)_{net} = -D \frac{dC_b}{dx}$$

$$\frac{dC_b}{dx} = -\frac{\left(\frac{N_b}{A}\right)_{net}}{D} \quad (3)$$

Substitute (2) and (3) into (1)

$$\frac{dC_a}{dx} = -\frac{dC_b}{dx}$$

$$-\frac{\left(\frac{N_a}{A}\right)_{net}}{D} = -\frac{\left(\frac{N_b}{A}\right)_{net}}{D}$$

$$-N_a = N_b \text{ or } N_a = -N_b$$

**Equimolar Counter Diffusion**



$$\left(\frac{N_a}{A}\right)_{net} = -D \frac{dC_a}{dx}$$

In terms of partial pressure, assume that the model gas behaves ideally

$$PV = nRT; \quad P_t V_t = nRT$$

For substance a:  $P_a = \frac{n_a RT}{V}$

$$\frac{P_a}{RT} = C_a; \quad P_a = C_a RT$$

$$dP_a = RT dC_a$$

$\therefore dC_a = \frac{dP_a}{RT}$  Substitute this equation into  $\left(\frac{N_a}{A}\right)_{net} = -D \frac{dC_a}{dx}$

Then  $\left(\frac{N_a}{A}\right)_{net} = -D \frac{dP_a/RT}{dx} = -D \frac{dP_a}{RT dx}$

For substance b:  $P_b = \frac{n_b RT}{V}$

Following the same procedure

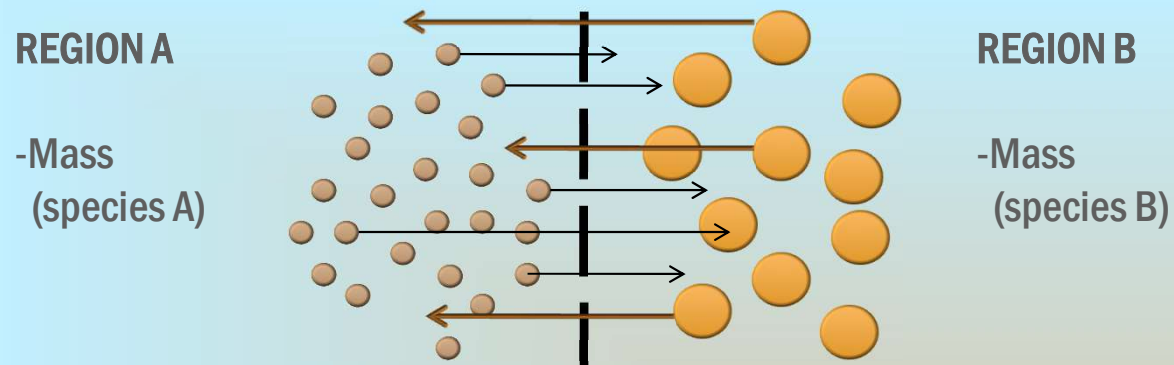
One can easily obtain:

$$\left(\frac{N_b}{A}\right)_{net} = -D \frac{dP_b}{RT dx}$$



# Heat, Mass, and Momentum Transport

## MASS TRANSPORT: (ECD)



### Generalizations:

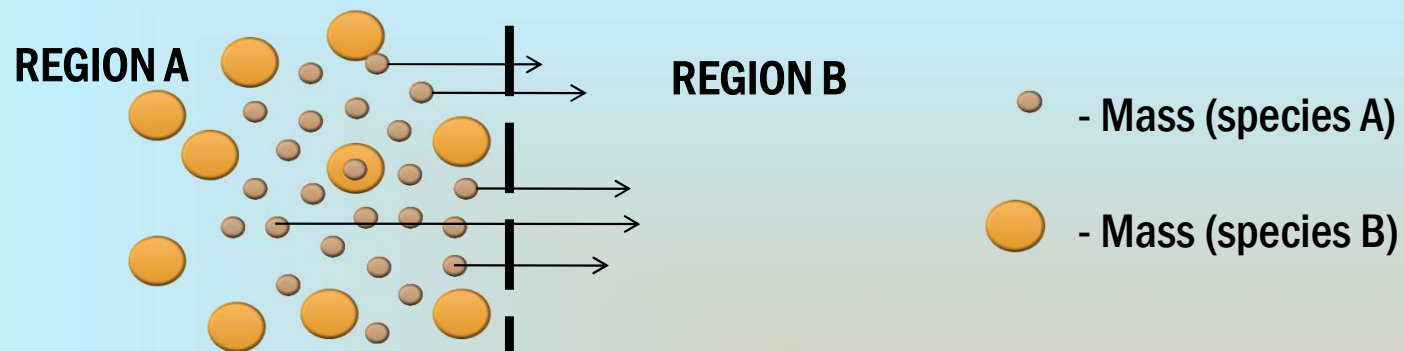
In ECD, component A diffuses at a rate through component B, which is also diffusing at the same molar rate as A, but in opposite direction.

$$\overline{N}_a = -\overline{N}_b$$



## Heat, Mass, and Momentum Transport

### MASS TRANSPORT: Diffusion Through Stationary Medium (DTSM)



#### Generalizations:

The boundary of the system is permeable to **only one component**.

Equation is based on the total mass transfer of both components in the system.



## Derivation of Mass Transfer Equation Through Stationary Gas

Definition of terms:

$(N_A)_t$  = total mass transfer rate of A

$(N_B)_t$  = total mass transfer rate of B

$(N_A)_b$  = bulk flow rate of A

$(N_B)_b$  = bulk flow rate of B

$(N_A)_m$  = molecular transport rate of A

$(N_B)_m$  = molecular transport rate of B

B – stationary gas

gas impermeable to the interphase



At any point the total mass transfer rate of A is:

$$(N_A)_t = (N_A)_b + (N_A)_m$$

Dividing by A = transfer area

$$\left(\frac{N_A}{A}\right)_t = \left(\frac{N_A}{A}\right)_b + \left(\frac{N_A}{A}\right)_m$$

For component B

$$(N_B)_t = (N_B)_b + (N_B)_m$$

$$\left(\frac{N_B}{A}\right)_t = \left(\frac{N_B}{A}\right)_b + \left(\frac{N_B}{A}\right)_m$$

Since B is a stationary gas, then  $\left(\frac{N_B}{A}\right)_t = 0$

$$\text{Then } \left(\frac{N_B}{A}\right)_b = -\left(\frac{N_B}{A}\right)_m$$

At constant T and P:

$$\left(\frac{N_A}{N_B}\right)_b = \frac{C_A}{C_B}$$

$$(N_A)_b = \frac{C_A}{C_B} (N_B)_b$$

Divide both sides by A:

$$\left(\frac{N_A}{A}\right)_b = \frac{C_A}{C_B} \left(\frac{N_B}{A}\right)_b$$





Also:  $\left(\frac{N_A}{A}\right)_b = \frac{C_A}{C_B} \left(-\frac{N_B}{A}\right)_m$

Since ECD applies on the bulk gas, then

$$\left(\frac{N_A}{A}\right)_m = -\left(\frac{N_B}{A}\right)_m$$

Substitute this equation into the above equation

$$\begin{aligned}\left(\frac{N_A}{A}\right)_b &= -\frac{C_A}{C_B} \left(-\frac{N_A}{A}\right)_m \\ \left(\frac{N_A}{A}\right)_b &= \frac{C_A}{C_B} \left(\frac{N_A}{A}\right)_m\end{aligned}$$

Substitute this equation into the total mass transfer rate of B divided by area will give:

$$\left(\frac{N_A}{A}\right)_t = -\frac{C_A}{C_B} \left(\frac{N_A}{A}\right)_m + \left(\frac{N_A}{A}\right)_m$$

Simplifying:

$$\begin{aligned}\left(\frac{N_A}{A}\right)_t &= -\left(\frac{C_A}{C_B} + 1\right) \left(\frac{N_A}{A}\right)_m \\ \left(\frac{N_A}{A}\right)_t &= -\left(\frac{C_A + C_B}{C_B}\right) \left(\frac{N_A}{A}\right)_m\end{aligned}$$

Since  $C_t = C_A + C_B$

Substituting:

$$\left(\frac{N_A}{A}\right)_t = \left(\frac{C_t}{C_B}\right) \left(\frac{N_A}{A}\right)_m$$

Since  $\left(\frac{N_A}{A}\right)_m = -D \frac{dC_A}{dx}$



By substituting

$$\left(\frac{N_A}{A}\right)_t = -D \frac{C_t}{C_B} \frac{dC_A}{dx}$$

Where  $C_t = \frac{P_t}{RT}$      $C_A = \frac{P_A}{RT}$      $C_B = \frac{P_B}{RT}$

$$\left(\frac{N_A}{A}\right)_t = -D \frac{\frac{P_t}{RT}}{\frac{P_B}{RT}} \frac{d\frac{P_A}{RT}}{dx}$$

$$\left(\frac{N_A}{A}\right)_t = -D \frac{P_t}{P_B} \frac{dP_A}{dx}$$



## Two Types of Mass Transport Mechanism

### 1. Equimolar Counter Diffusion (ECD)

- Component A diffuses through B which is diffusing at the same molar rate as A but in opposite direction
- The boundaries of the system are permeable to both components
- At constant T and P, both A and B will diffuse because of their concentration gradient

$$\left(\frac{N_a}{A}\right)_{net} = -D \frac{dC_a}{dx}$$

$$\left(\frac{N_b}{A}\right)_{net} = -D \frac{dC_b}{dx}$$

$$\frac{N_a}{A} = -D \frac{dP_a}{RTdx}$$

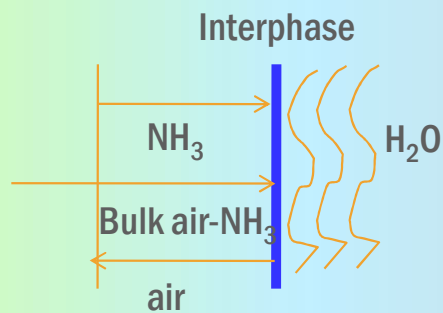
$$\frac{N_b}{A} = -D \frac{dP_b}{RTdx}$$



## Two Types of Mass Transport Mechanism

### 2. Diffusion through a Stationary Medium (DSTM)

- Occurs when one boundary of the system is permeable to only one component
- Example: Absorption of  $\text{NH}_3$  from  $\text{NH}_3$ -air mixture by  $\text{H}_2\text{O}$



The bulk flow of air is equal to molecular flow

$$(N_{\text{air}})_{\text{bulk}} = (N_{\text{air}})_{\text{molecular}}$$

$$\left(\frac{N_a}{A}\right)_t = -D \frac{C_t}{C_b} \frac{dC_a}{dx}$$

$$\left(\frac{N_a}{A}\right)_t = -\frac{D}{RT} \frac{P_t}{P_b} \frac{dP_a}{dx}$$



# Momentum Transport

- Transport of momentum if there are differences in velocity

$$\tau_{yx} = \frac{F_y}{A} g_c = -\mu \frac{dv_y}{dx}$$

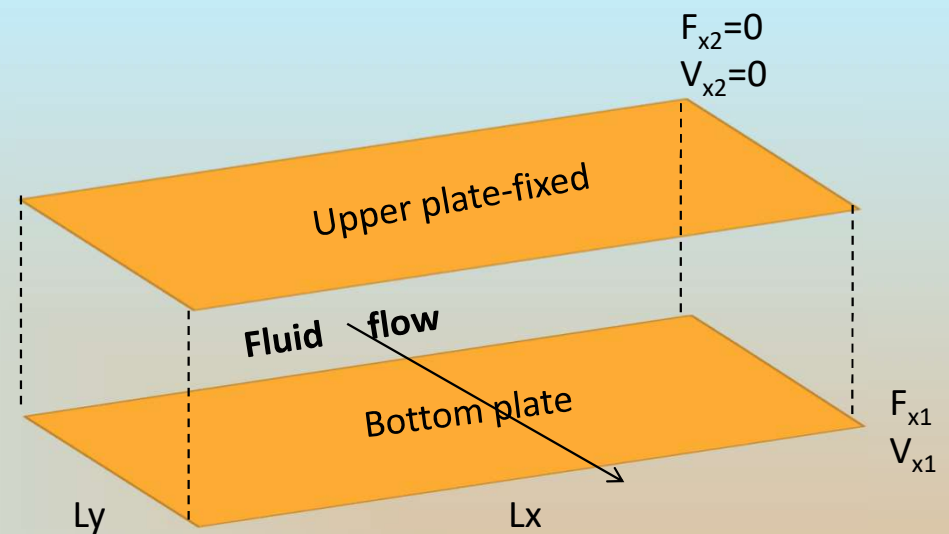
where :  $\tau_{yx}$  momentum flux (kg/m.s<sup>2</sup>)

y direction of flow or velocity

x direction of momentum flux

$\mu$  absolute viscosity (kg/m.s)

$\frac{dv_y}{dx}$  velocity gradient along x (m/s/m)



# Momentum Transport

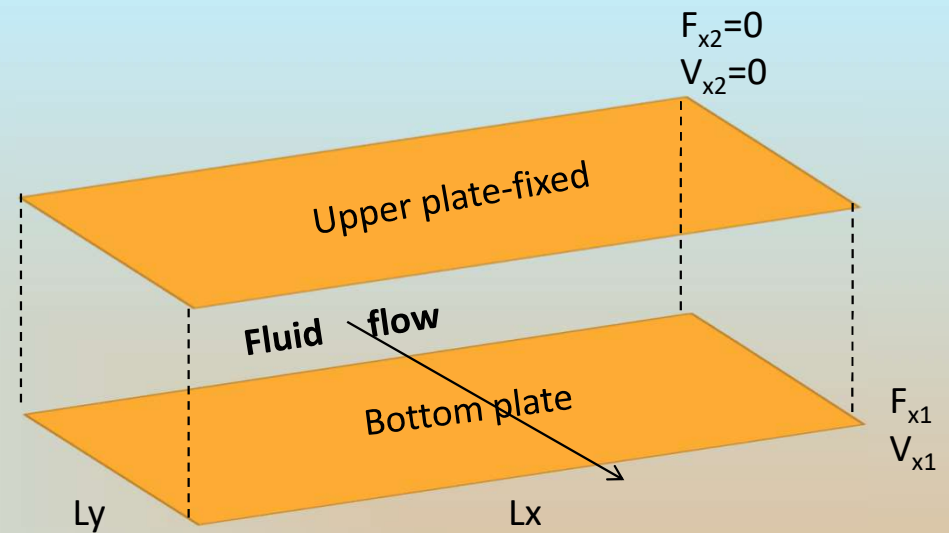
$\frac{F_y}{A}$  shear stress (N/m<sup>2</sup>)

$g_c$  gravitational acceleration (kg.m/N.s<sup>2</sup>)

From Newton' s 2<sup>nd</sup> Law

$$F_y = m \cdot a \quad \text{and} \quad a = \frac{d\bar{v}}{dt}$$

$$F_y = m \frac{d\bar{v}}{dt} \rightarrow \frac{F_y}{A} = \frac{d(m\bar{v})}{dt}$$



## SUMMARY

From the three laws, an analogy was developed with respect to the ultrasimplified kinetic theory of gases.

$$\Psi = \frac{-lc}{6} \left( \frac{d\Gamma}{dx} \right) = -\delta \frac{d\Gamma}{dx}$$

where:  $\delta$  – proportionality constant

$$Q = \frac{q}{A} = -k \frac{dT}{dx}$$

$$\frac{\overline{N}_a}{A} = -D \frac{dC_a}{dx}$$

$$\tau_{yx} = \frac{F_y}{A} g_c = -\mu \frac{dv_y}{dx}$$



## Analogous Form of Molecular Transport Equations

General	Mass	Heat	Momentum
$\psi$	Na	Q	$\tau_{yx}$
$\delta$	D	$\alpha$	$\nu$
$\Gamma$	mass/vol or mol/vol	$\rho c_p T$	$\rho v_y$
$\frac{d\Gamma}{dx}$	$\frac{dC_a}{dx}$	$\frac{d\rho c_p T}{dx}$	$\frac{d\rho v_y}{dx}$
Phenomenological Equation	Fick's law of molecular diffusion	Fourier's law of heat conduction	Newton's law of viscosity
Diffusivity	$D = D$	$k = \rho c_p T$	$M = \rho \nu_y$
Ratio of Diffusivities			
	Momentum/mass	Momentum/thermal	Thermal/mass
	$\frac{\nu}{D} = \frac{\mu}{\rho D} = N_{sc}$	$\frac{\nu}{\alpha} = \frac{\mu c_p}{k} = N_{sc}$	$\frac{\alpha}{D} = \frac{k}{\rho c_p D} = \frac{N_{sc}}{N_{pr}} = N_{le}$
Dimensionless number	Schmidt number	Prandtl number	Lewis number



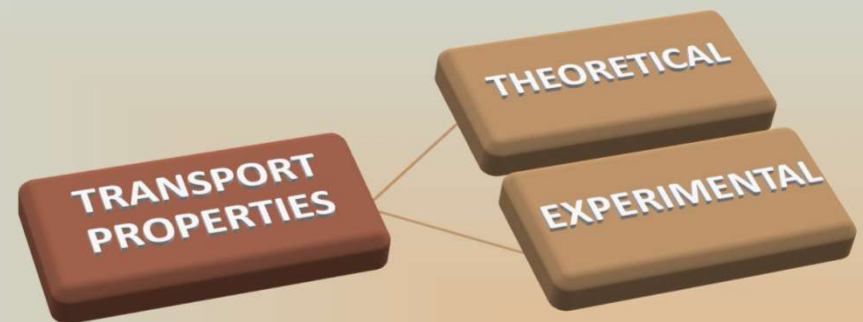


# TRANSPORT PROPERTIES OF GASES, LIQUIDS, AND SOLIDS

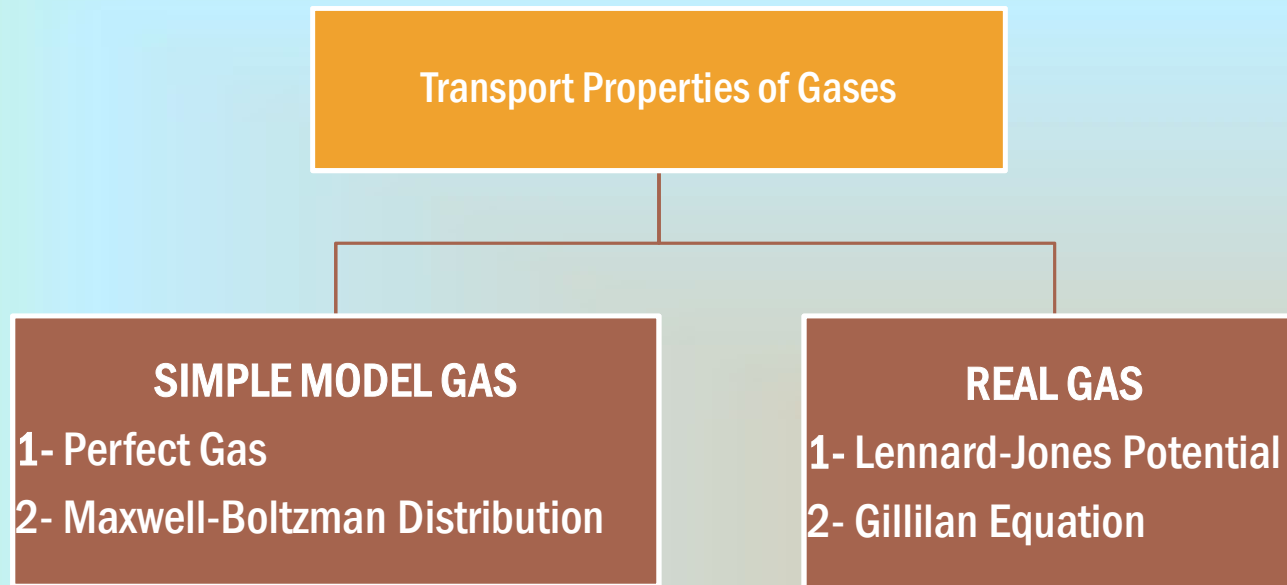


# TRANSPORT PROPERTIES

- The general term transport properties includes the **mass diffusivity, thermal conductivity, and absolute viscosity** of gases liquids, and solids.
- Obtained from the derivation of relationships for the mean path,  $l$  and mean speed,  $c$  (**theoretical**) and the consideration of forces acting between molecules (**experimental**).
- The general term “transport properties” includes the mass diffusivity, thermal conductivity, and absolute viscosity of gases liquids, and solids.



# Transport Properties of GASES



## TRANSPORT PROPERTIES OF GASES

### SIMPLE MODEL GAS

- Basically, derived from the kinetic theory of gases which derives for expressions of **mean path,  $l$**  and **mean speed,  $c$**  under ideal assumptions
- Assumptions:
  1. Molecule is a perfect sphere
  2. No attraction and repulsion between particles
  3. Volume of particle is very small compared to the volume of the space between molecules
  4. Exact collision between molecules



## SIMPLE MODEL GAS

### Mean Speed

- By ideal gas law

$$\bar{c} = \left( \frac{3RT}{M} \right)^{1/2}$$

- By Maxwell-Boltzmann distribution

$$\bar{c} = \left( \frac{8RT}{\mu M} \right)^{1/2}$$

where:

- R = ideal gas constant
- T = absolute Temperature
- M = molecular weight



## SIMPLE MODEL GAS

### Mean Free Path

- By ideal gas law

$$l = \frac{RT}{\left(\frac{1}{2} + \frac{3}{2}\sqrt{2}\right) \bar{A} P \pi \sigma^2}$$

- By Maxwell-Boltzmann distribution

$$l = \frac{RT}{(\sqrt{2}) \bar{A} P \pi \sigma^2}$$

where:

- P = pressure
- T = absolute Temperature
- M = molecular weight
- $\bar{A}$  = Avogadro's
- $\sigma$  = molecular diameter



## Elastic-Sphere Equivalent Diameter

Gas	$\sigma, 10^{-8} \text{ cm}$	Gas	$\sigma, 10^{-8} \text{ cm}$
H <sub>2</sub>	2.74	C <sub>2</sub> H <sub>6</sub>	5.3
Ne	3.75	O <sub>2</sub>	3.61
CH <sub>4</sub>	4.14	HCl	4.46
NH <sub>3</sub>	4.43	A	3.64
H <sub>2</sub> O	4.6	CO <sub>2</sub>	4.59
N <sub>2</sub>	3.75	Kr	4.16
C <sub>2</sub> H <sub>4</sub>	4.95	Xe	4.85



## SIMPLE MODEL GAS

### Diffusivity Constant

- For gases with sufficiently low densities

$$P_r = \frac{P}{P_c} < 0.6, \quad T_r = \frac{T}{T_c} > 1.3$$

### Mass Diffusivity

$$D = \frac{4.81 \times 10^{-24} T^{3/2}}{P \sigma^2 M^{1/2}}$$

### Thermal Conductivity

- Note:  $k = \alpha \rho c_p$      $\rho = \frac{PM}{RT}$      $C_p = \frac{5}{2} \left( \frac{R}{M} \right)$

$$k = \frac{1.203 \times 10^{-2} (TM)^{1/2}}{\sigma^2} \quad (\text{mole basis}) \quad k = \frac{1.203 \times 10^{-23} (T/M)^{1/2}}{\sigma^2} \quad (\text{mass basis})$$





## SIMPLE MODEL GAS

For gases with sufficiently low densities

### Absolute Viscosity

- Note:  $\mu = \nu \rho$      $\rho = \frac{PM}{RT}$

$$\mu = \frac{5.79 \times 10^{-25} (MT)^{1/2}}{\sigma^2}$$

- The transport properties using the simple model gas,  $\sigma$  has no real physical meaning and it cannot be measured directly. Instead it must be determined from some measurable property, such as the viscosity
  - ✓ Relationship of  $k$  and  $\mu$      $k = \frac{5\rho\mu}{2M}$
  - ✓ Relationship of  $D$  and  $\mu$      $D = \frac{\mu}{\rho}$



## REAL GASES

- Lennard-Jones Potential – valid for non-polar molecules only
- Evaluated from the concept of collision diameter

$$\sigma_{ab} = \frac{1}{2}(\sigma_a + \sigma_b)$$

- Potential parameters are also considered

$$\frac{\varepsilon_{ab}}{k} = \sqrt{\frac{\varepsilon_a}{k} \frac{\varepsilon_b}{k}}; \varepsilon \text{ is the energy constant}$$

with corresponding collision integral,  $\Omega$

$$T_{ab}^* = \frac{kT}{\varepsilon_{ab}}$$



## Constants for Lennard-Jones Potential

Species	$\varepsilon/k_B$ (K)	$\sigma$ (Å)
He	10.22	2.56
Ne	35.6	2.75
Ar	120	3.40
Kr	171	3.60
Xe	220	4.10
N <sub>2</sub>	95.5	3.74
CH <sub>4</sub>	148.4	3.81
CF <sub>4</sub>	151.4	4.75
H <sub>2</sub>	39.4	2.81
O <sub>2</sub>	118	3.58
CO	100	3.76
CO <sub>2</sub>	309	3.36
C <sub>2</sub> H <sub>4</sub>	470	2.5
C <sub>2</sub> H <sub>6</sub>	243	3.95
C <sub>3</sub> H <sub>8</sub>	242	5.64
C(CH <sub>3</sub> ) <sub>4</sub>	232	7.44
C <sub>6</sub> H <sub>6</sub>	830	3.4
C <sub>6</sub> H <sub>6</sub> -CH <sub>4</sub> O	1018.2	2.896
C <sub>6</sub> H <sub>6</sub> -C <sub>2</sub> H <sub>6</sub> O	553.5	4.651
C <sub>6</sub> H <sub>6</sub> -C <sub>3</sub> H <sub>6</sub> O	632.1	4.620
C <sub>6</sub> H <sub>6</sub> -C <sub>4</sub> H <sub>10</sub> O	1122.3	3.425



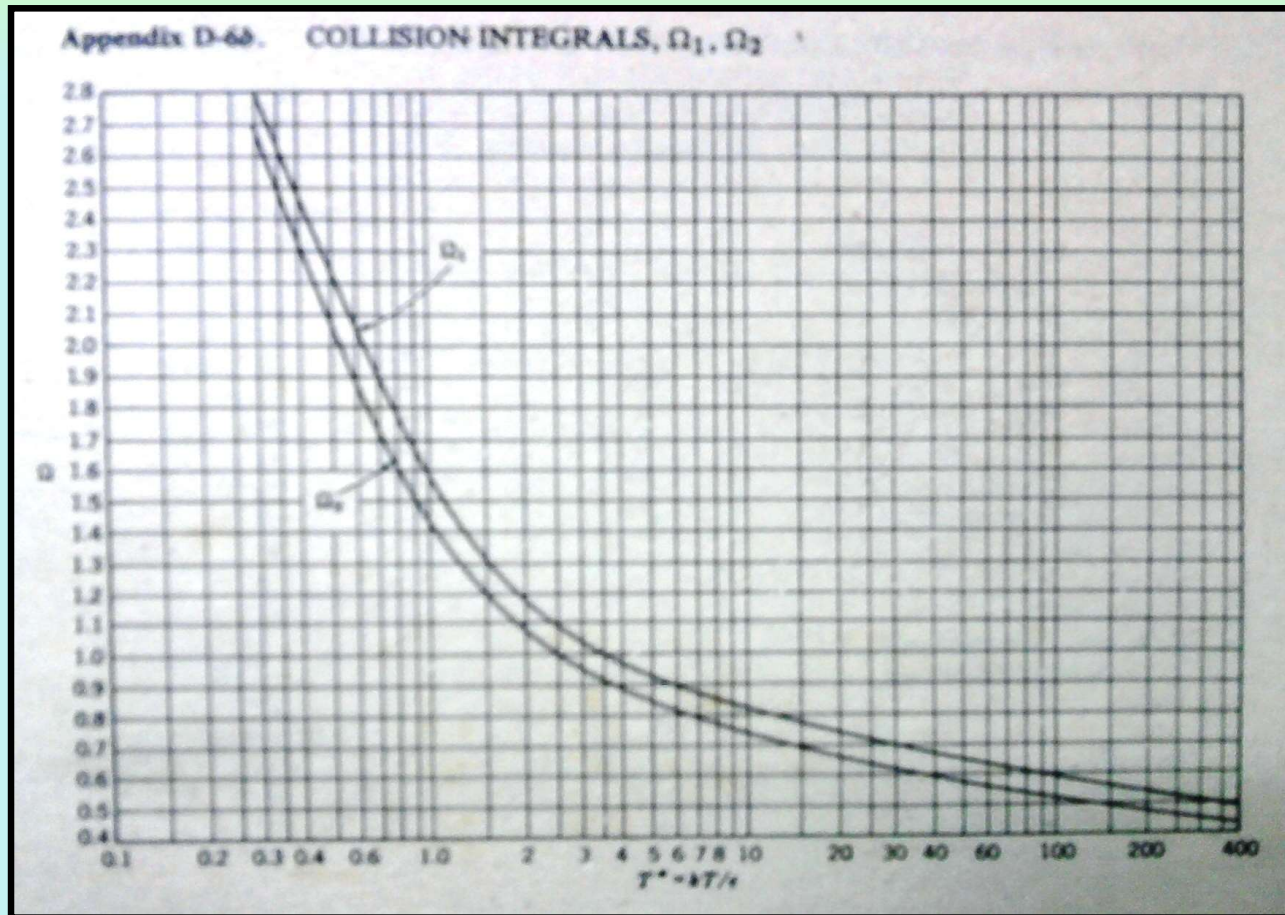
## Constants for Lennard-Jones Potential

Lennard-Jones (12-6) potential parameters.

Non-polar molecules	$\sigma$ (Å)	$b_0$ (cal/mol <sup>-1</sup> atm <sup>-1</sup> )	$\varepsilon/k_B$ (K)
H <sub>2</sub>	2.92	0.760	37.02
N <sub>2</sub>	3.72	1.572	94.50
O <sub>2</sub>	3.58	1.401	117.5
Cl <sub>2</sub>	4.115	2.128	357
N <sub>2</sub> O	3.88	1.789	232.4
CO <sub>2</sub>	3.967	1.906	208.1
CH <sub>4</sub>	3.82	1.702	148
C <sub>2</sub> H <sub>2</sub>	4.22	2.29508	185
AsH <sub>3</sub>	4.06	2.044	281
C <sub>6</sub> H <sub>6</sub>	5.27	4.469	440
Br <sub>2</sub>	3.86	1.75639	400
COS	4.13	2.151	335
C <sub>2</sub> N <sub>2</sub>	4.38	2.566	339
CH <sub>2</sub>	4.23	2.314	205
HCl	3.31	1.1075	360
I <sub>2</sub>	4.98	3.77179	550
SO <sub>2</sub>	4.29	2.411	252
A	3.41	1.211	119.5
He	2.63	0.556	6.03
Ne	2.74	0.628	35.7
Kr	3.61	1.437	190
Xe	4.05	2.03	230
Air	3.62	1.44872	97.0



## Collision Integrals



## REAL GASES

### Lennard-Jones Potential

- Absolute Viscosity

$$\mu = \frac{8.42 \times 10^{-25} (MT)^{1/2}}{\sigma^2 \Omega_1}$$

For multicomponent gas mixtures at low density

$$\mu_{mix} = \sum_{i=1}^n \frac{x_i \mu_i}{\sum_{j=1}^n x_j \Phi_{ij}}$$

$$\Phi_{ij} = \frac{1}{\sqrt{8}} \left( 1 + \frac{M_i}{M_j} \right)^{-1/2} \left[ 1 + \left( \frac{\mu_i}{\mu_j} \right)^{1/2} \left( \frac{M_i}{M_j} \right)^{1/4} \right]^2$$



## REAL GASES

### Lennard-Jones Potential

### Thermal Conductivity

$$k = \frac{2.63 \times 10^{-23} \left(T/M\right)^{1/2}}{\sigma^2 \Omega_1}$$

### Relationship of $k$ and $\mu$

For monoatomic (noble gases He, Ar, Xe) gases:  $k = \frac{15R\mu}{4M}$

For polyatomic ( $N_2$ ,  $O_2$ ) gases:  $k = \frac{15R\mu}{4M} \left( \frac{4C_v}{15} + \frac{3}{5} \right)$



## REAL GASES

### Lennard-Jones Potential

- Mass Diffusivity

$$D_{ab} = \frac{8.42 \times 10^{-247} \sqrt{T^3 \left(\frac{1}{2}\right) \left(\frac{1}{M_a} + \frac{1}{M_b}\right)}}{P \sigma_{ab}^2 \Omega_2}$$

For gas mixture of several components:

$$D_{1-mixtur} = \frac{1}{\frac{y_2}{D_{1-2}} + \frac{y_3}{D_{1-3}} + \dots + \frac{y_n}{D_{1-n}}}$$

- Gilliland Equation – valid for many gases

$$D_{ab} = \frac{1.38 \times 10^{-7} \sqrt{T^3 \left(\frac{1}{M_a} + \frac{1}{M_b}\right)}}{P \left(V_a^{1/3} + V_b^{1/3}\right)^2}$$

where V is the molar volume.

- ✓ The term  $V^{1/3}$  is a measure of the molecular diameter of each constituent and is analogous to  $\sigma$ .





## Atomic Volumes for Use In Calculating the Molar Volume at the Normal Boiling Point

**Appendix D-7. ATOMIC VOLUMES FOR USE IN CALCULATING THE MOLAR VOLUME AT THE NORMAL BOILING POINT**  
(Le Bas, *The Molecular Volumes of Liquid Chemical Compounds*, By permission of Longmans, copyright 1915)

Element	Atomic Volume cm <sup>3</sup> /g atom
Air	29.9
Antimony	34.2
Arsenic	30.5
Bismuth	48.0
Bromine	27.0
Carbon	14.8
Chlorine, terminal as R-CL	21.6
medial as R-CHCl-R	24.6
Chromium	27.4
Fluorine	8.7
Germanium	34.5
Hydrogen, in compounds	3.7
as hydrogen molecule	7.15
Iodine	37.0
Lead	46.5-50.1
Mercury	19.0
Nitrogen	15.6
in primary amines	10.5
in secondary amines	12.0
Oxygen, doubly bound as -C=O	7.4
Coupled to two other elements:	
in aldehydes and ketones	7.4
in methyl ethers	9.9
in methyl esters	9.1
in higher ethers and esters	11.0
in acids	12.0
in union with S, P, N	8.3
Phosphorus	27.0
Silicon	32.0
Sulfur	25.6
Tin	42.3
Titanium	35.7
Vanadium	32.0
Water	18.8
Zinc	20.4
For 3-membered ring, as in ethylene oxide	-6
For 4-membered ring, as in cyclobutane	-8.5
For 5-membered ring, as in furan	-11.5
For six-membered ring, as in benzene, cyclohexane	-15
For naphthalene ring	-30
For anthracene ring	-47.5



## TRANSPORT PROPERTIES OF LIQUIDS

- The kinetic theory of liquids is not well organized and no single theory has been generally accepted.
- Liquids have complex structure and since the molecules are close together, therefor the intermolecular forces are strong.

### EYRING SIMPLE “HOLE” MODEL

- **Molecular Migration**

A molecule may migrate into a neighboring hole, provided that enough force is available to overcome IMFA

- **Molecular Vibration/Collision**

The molecule vibrates within a limited space confined by the forces of neighboring molecules.



## EYRING SIMPLE “HOLE” MODEL

- Applicable for short temperature ranges.

### Absolute Viscosity

$$\mu = C e^{\left(\frac{B}{RT}\right)}$$

- When no viscosity data is available:

$$\mu = \frac{4 \times 10^{-10} e^{\frac{3.8T_b}{T}}}{V}$$

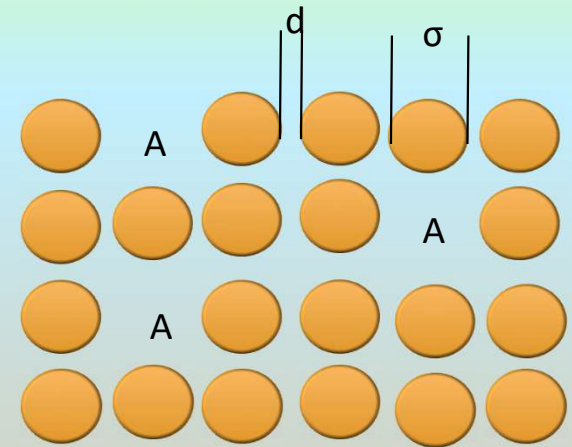
where:

T = temperature, K

B and C are constants

V = molar volume, m<sup>3</sup>/mol

T<sub>b</sub> = normal boiling point



*To cause “flow” in a liquid, a relatively large force must be applied to overcome the strong IMFA tending to hold molecules in place*



## EYRING SIMPLE “HOLE” MODEL

Applicable for short temperature ranges.

### Thermal Conductivity

$$k = 3.59 \times 10^{-9} C_p \rho \left( \frac{\rho}{M} \right)^{1/3}$$

where:

$K$  = thermal conductivity, J/s-m-°C

$C_p$  = heat capacity, J/kg-°C

$M$  = molecular weight, kg/mol

$\rho$  = density, kg/m<sup>3</sup>

### Mass Diffusivity

$$\frac{T}{D\mu} = \frac{1}{AC} = F$$

where:

$D$  = mass diffusivity m<sup>2</sup>/s

$F$  = function of molar volume



# TRANSPORT PROPERTIES OF SOLIDS

## Structures

1. Crystalline – atoms are arranged in a regular pattern called a crystal lattice as in metals and salts
2. Amorphous – do not have a crystal lattice although they do have some order to their arrangement of atoms, e.g. glass, plastics, paint, rubber

Diffusivities in solids  
at 1 atm.

SYSTEM	TEMPERATURE, °C	D, m <sup>2</sup> /s
H <sub>2</sub> in Ni	400	$0.95 \times 10^{-10}$
H <sub>2</sub> in Pd	400	$0.316 \times 10^{-6}$
O <sub>2</sub> in Ag	400	$0.32 \times 10^{-12}$
CO in mild steel	400	$0.67 \times 10^{-8}$
He in SiO <sub>2</sub>	400	$0.81 \times 10^{-16}$
Au in Ag	870	$0.43 \times 10^{-13}$
Ni in Cu	400	$0.23 \times 10^{-12}$



## SUMMARY of TRANSPORT PROPERTIES

### Determination of Gas Phase Diffusivity

1. Equations and Correlations for Gas Diffusivity: Tables 5-13, 5-14, 5-15, 5-16 (PCEH 7<sup>th</sup> ed.)
2. Diffusivities of pairs of gases and vapors: Table 2-371 (PCEH 7<sup>th</sup> ed.)

### Determination of Liquid Phase Diffusivity

1. Correlations and diffusivities of dilute, binary mixture of non-electrolyte liquids: Table 5-18 (PCEH 7<sup>th</sup> ed.)
2. Diffusivities of Liquids at 25 °C: Table 2-372 (PCEH 7<sup>th</sup> ed.)

### Determination of Viscosities of Gases and Liquids

- Table 2-364 and Table 2-365 (PCEH 7<sup>th</sup> ed.)



**TABLE 5-13 Rules of Thumb for Diffusivities (See Cussler, Reid et al., Schwartzberg and Chao)**

Continuous phase	$D_i$ magnitude		$D_i$ range		Comments
	m <sup>2</sup> /s	cm <sup>2</sup> /s	m <sup>2</sup> /s	cm <sup>2</sup> /s	
Gas at atmospheric pressure	10 <sup>-5</sup>	0.1	10 <sup>-4</sup> –10 <sup>-6</sup>	1–10 <sup>-2</sup>	Accurate theories exist, generally within $\pm 10\%$ ; $D_i P \approx \text{constant}$ ; $D_i \propto T^{1.66 \text{ to } 2.0}$
Liquid	10 <sup>-9</sup>	10 <sup>-5</sup>	10 <sup>-8</sup> –10 <sup>-10</sup>	10 <sup>-4</sup> –10 <sup>-6</sup>	Approximate correlations exist, generally within $\pm 25\%$
Liquid occluded in solid matrix	10 <sup>-10</sup>	10 <sup>-6</sup>	10 <sup>-8</sup> –10 <sup>-12</sup>	10 <sup>-4</sup> –10 <sup>-8</sup>	Hard cell walls: $D_{\text{eff}}/D_i = 0.1$ to $0.2$ . Soft cell walls: $D_{\text{eff}}/D_i = 0.3$ to $0.9$
Polymers and glasses	10 <sup>-12</sup>	10 <sup>-8</sup>	10 <sup>-10</sup> –10 <sup>-14</sup>	10 <sup>-6</sup> –10 <sup>-10</sup>	Approximate theories exist for dilute and concentrated limits; strong composition dependence
Solid	10 <sup>-14</sup>	10 <sup>-10</sup>	10 <sup>-10</sup> –10 <sup>-34</sup>	10 <sup>-6</sup> –10 <sup>-30</sup>	Approximate theories exist; strong temperature dependence

**TABLE 5-14 Correlations of Diffusivities for Gases**

Authors*	Equation	Error
1. Binary Mixtures—Low Pressure—Nonpolar		
Chapman-Enskog	$D_{AB} = \frac{0.001858 T^{3/2} M_{AB}^{1/2}}{P \sigma_{AB}^2 \Omega_D} \quad (5-194)$	7.3%
Wilke-Lee [65]	$D_{AB} = \frac{(0.0027 - 0.0005 M_{AB}^{1/2}) T^{3/2} M_{AB}^{1/2}}{P \sigma_{AB}^2 \Omega_D} \quad (5-195)$	7.0%
Fuller-Schettler-Giddings [19]	$D_{AB} = \frac{0.001 T^{1.75} M_{AB}^{1/2}}{P [(\sum v)_A^{1/3} + (\sum v)_B^{1/3}]^2} \quad (5-196)$	5.4%
2. Binary Mixtures—Low Pressure—Polar		
Brokaw [4]	$D_{AB} = \frac{0.001858 T^{3/2} M_{AB}^{1/2}}{P \sigma_{AB}^2 \Omega_D} \quad (5-197)$	9.0%



**TABLE 5-15 Estimates for  $\varepsilon_i$  and  $\sigma_i$  (K, Å, atm, cm<sup>3</sup>, mol)**

Critical point	$\varepsilon/k = 0.75 T_c$	$\sigma = 0.841 V_c^{1/3}$ or $2.44 (T_c/P_c)^{1/3}$
Critical point	$\varepsilon/k = 65.3 T_c z_c^{3.6}$	$\sigma = \frac{1.866 V_c^{1/3}}{z_c^{1.2}}$
Normal boiling point	$\varepsilon/k = 1.15 T_b$	$\sigma = 1.18 V_b^{1/3}$
Melting point	$\varepsilon/k = 1.92 T_m$	$\sigma = 1.222 V_m^{1/3}$
Acentric factor	$\varepsilon/k = (0.7915 + 0.1693 \omega) T_c$	$\sigma = (2.3551 - 0.087 \omega) \left( \frac{T_c}{P_c} \right)^{1/3}$

NOTE: These values may not agree closely, so usage of a consistent basis is suggested (e.g., data at the normal boiling point).

**TABLE 5-16 Atomic Diffusion Volumes for Use in Estimating  $D_{AB}$  by the Method of Fuller, Schettler, and Giddings**

Atomic and Structural Diffusion-Volume Increments, $v_i$ (cm <sup>3</sup> /mol)			
C	16.5	(Cl)	19.5
H	1.98	(S)	17.0
O	5.48	Aromatic ring	-20.2
(N)	5.69	Heterocyclic ring	-20.2
Diffusion Volumes for Simple Molecules, $\Sigma v_i$ (cm <sup>3</sup> /mol)			
H <sub>2</sub>	7.07	CO	18.9
D <sub>2</sub>	6.70	CO <sub>2</sub>	26.9
He	2.88	N <sub>2</sub> O	35.9
N <sub>2</sub>	17.9	NH <sub>3</sub>	14.9
O <sub>2</sub>	16.6	H <sub>2</sub> O	12.7
Air	20.1	(CCl <sub>2</sub> F <sub>2</sub> )	114.8
Ar	16.1	(SF <sub>6</sub> )	69.7
Kr	22.8	(Cl <sub>2</sub> )	37.7
(Xe)	37.9	(Br <sub>2</sub> )	67.2
Ne	5.59	(SO <sub>2</sub> )	41.1

Parentheses indicate that the value listed is based on only a few data points.





**TABLE 2-371 Diffusivities of Pairs of Gases and Vapors (1 atm)** $D_e$  in  $\text{cm}^2/\text{s}$ 

Substance	Temp., °C	Air	A	H <sub>2</sub>	O <sub>2</sub>	N <sub>2</sub>	CO <sub>2</sub>	N <sub>2</sub> O	CH <sub>4</sub>	C <sub>2</sub> H <sub>6</sub>	C <sub>2</sub> H <sub>4</sub>	<i>n</i> -C <sub>4</sub> H <sub>10</sub>	<i>i</i> -C <sub>4</sub> H <sub>10</sub>	Ref.
Acetic acid	0	0.1064		0.416			0.0716							8
Acetone	0	.109		.361										6, 16
<i>n</i> -Amyl alcohol	0	.0589		.235			.0422							8
<i>sec</i> -Amyl alcohol	30	.072												5
Amyl butyrate	0	.040												8
Amyl formate	0	.0543												8
<i>t</i> -Amyl formate	0	.058												8
Amyl isobutyrate	0	.0419		.171										8
Amyl propionate	0	.046		.1914			.0347							8
Aniline	0	.0610												8
	30	.075												5
Anthracene	0	.0421												8
Argon	20					0.194								18
Benzene	0	.077		.306	0.0797		.0528							8, 15
Benzidine	0	.0298												8
Benzyl chloride	0	.066												8
<i>n</i> -Butyl acetate	0	.058												8
<i>i</i> -Butyl acetate	0	.0612		.2364			.0425							8
<i>n</i> -Butyl alcohol	0	.0703		.2716			.0476							8
	30	.088												5
<i>t</i> -Butyl alcohol	0	.0727		.2771			.0483							8
Butyl amine	0	.0821												8
<i>t</i> -Butyl amine	0	.0853												8



**TABLE 5-18 Correlations for Diffusivities of Dilute, Binary Mixtures of Nonelectrolytes in Liquids**

Authors*	Equation	Error
1. General Mixtures		
Wilke-Chang [64]	$D_{AB}^o = \frac{7.4 \times 10^{-8} (\phi_B M_B)^{1/2} T}{\mu_B V_A^{0.5}} \quad (5-208)$	20%
Tyn-Calus [59]	$D_{AB}^o = \frac{8.93 \times 10^{-8} (V_A/V_B^2)^{1/6} (\psi_B/\psi_A)^{0.6} T}{\mu_B} \quad (5-209)$	10%
Umes-Danner [60]	$D_{AB}^o = \frac{2.75 \times 10^{-8} (R_B/R_A^{2/3}) T}{\mu_B} \quad (5-210)$	16%
Siddiqi-Lucas [52]	$D_{AB}^o = \frac{9.89 \times 10^{-8} V_B^{0.265} T}{V_A^{0.45} \mu_B^{0.907}} \quad (5-211)$	13%
2. Gases in Low Viscosity Liquids		
Sridhar-Potter [54]	$D_{AB}^o = D_{BB} \left( \frac{V_{cB}}{V_{cA}} \right)^{2/3} \left( \frac{V_B}{V_{mB}} \right) \quad (5-212)$	18%
Chen-Chen [7]	$D_{AB}^o = 2.018 \times 10^{-9} \frac{(\beta V_{cB})^{2/3} (RT_{cB})^{1/2}}{M_A^{1/6} (M_B V_{cA})^{1/3}} (V_r - 1) \left( \frac{T}{T_{cB}} \right)^{1/2} \quad (5-213)$	6%



**TABLE 2-372 Diffusivities in Liquids (25°C)**

Dilute solutions and 1 atm unless otherwise noted; use  $D_L \mu/T = \text{constant}$  to estimate effect of temperature; \* indicates that reference gives effect of concentration.

Solute	Solvent	$D_L \times 10^5$ , sq cm/sec	Estimated possible, error, $\pm$ %1	Ref.
Acetal*	Ethanol	1.25	5	11
Acetamide*	Ethanol	0.68	5	11
Acetamide*	Water	1.19	3	11
Acetic acid	Acetone	3.31		4
Acetic acid	Benzene	2.11		1, 4
Acetic acid	Carbon tetrachloride	1.49		4
Acetic acid	Ethylene glycol	0.13		4
Acetic acid	Toluene	2.26		4
Acetic acid*	Water	1.24	3	11
Acetonitrile	Water	1.66	5	11
Acetylene	Water	1.78, 2.11		1, 24
Allyl alcohol*	Ethanol	1.06	5	11
Allyl alcohol	Water	1.19	6	11
Ammonia*	Water	1.7, 2.0, 2.3		1, 11
<i>t</i> -Amyl alcohol*	Ethanol	0.87	5	11
<i>t</i> -Amyl alcohol	Water	1.0	8	11, 25
Benzene	Carbon tetrachloride	1.53		7
Benzene (50 mole %)	<i>n</i> -Decane	1.72		26
Benzene (50 mole %)	2,4-Dimethyl pentane	2.49		26
Benzene (50 mole %)	<i>n</i> -Dodecane	1.40		26
Benzene (50 mole %)	<i>n</i> -Heptane	2.47		26
Benzene (50 mole %)	<i>n</i> -Hexadecane	0.96		26
Benzene (50 mole %)	<i>n</i> -Octadecane	0.86		26



TABLE 2-364 Viscosities of Gases: Coordinates for Use			
Gas	X	Y	$\mu \times 10^7$ p
Acetic acid	7.0	14.6	825 (50°C)
Acetone	8.4	13.2	735
Acetylene	9.3	15.5	1017
Air	10.4	20.4	1812
Ammonia	8.4	16.0	1000
Amylene ( $\beta$ )	8.6	12.2	676
Argon	9.7	22.6	2215
Arsine	8.6	20.0	1576
Benzene	8.7	13.2	746
Bromine	8.8	19.4	1495
Butane ( $n$ )	8.6	13.2	735
Butane (iso)	8.6	13.2	744
Butyl acetate (iso)	5.7	16.3	778
Butylene ( $\alpha$ )	8.4	13.5	761
Butylene ( $\beta$ )	8.7	13.1	746
Butylene (iso)	8.3	13.9	786
Butyl formate (iso)	6.6	16.0	840
Cadmium	7.8	22.5	5690 (500)
Carbon dioxide	8.9	19.1	1463
Carbon disulfide	8.5	15.8	990
Carbon monoxide	10.5	20.0	1749
Carbon oxysulfide	8.2	17.9	1220
Carbon tetrachloride	8.0	15.3	966

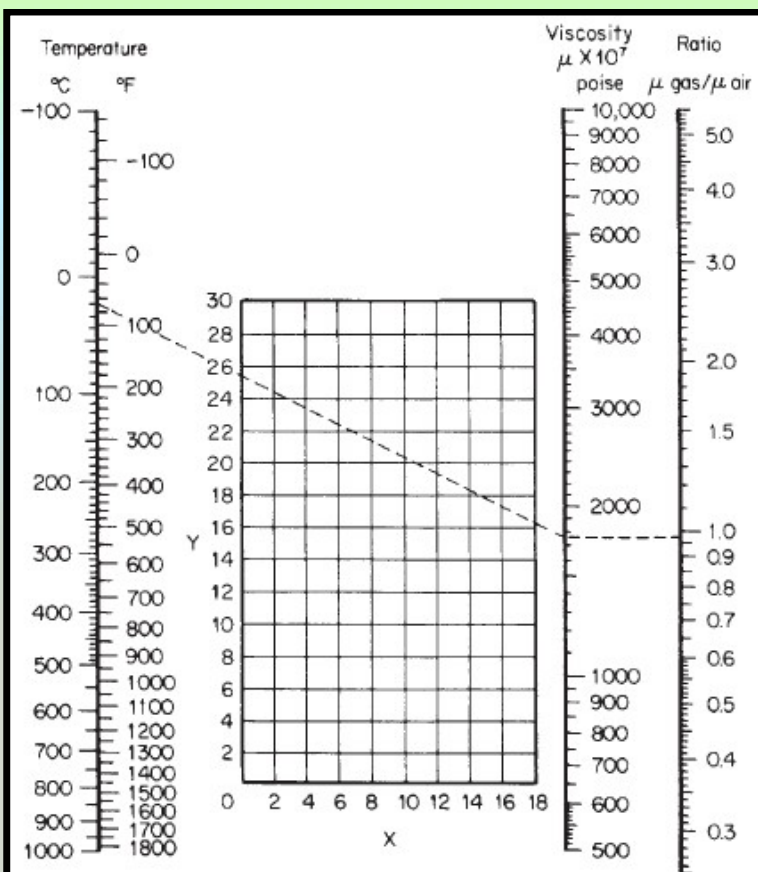
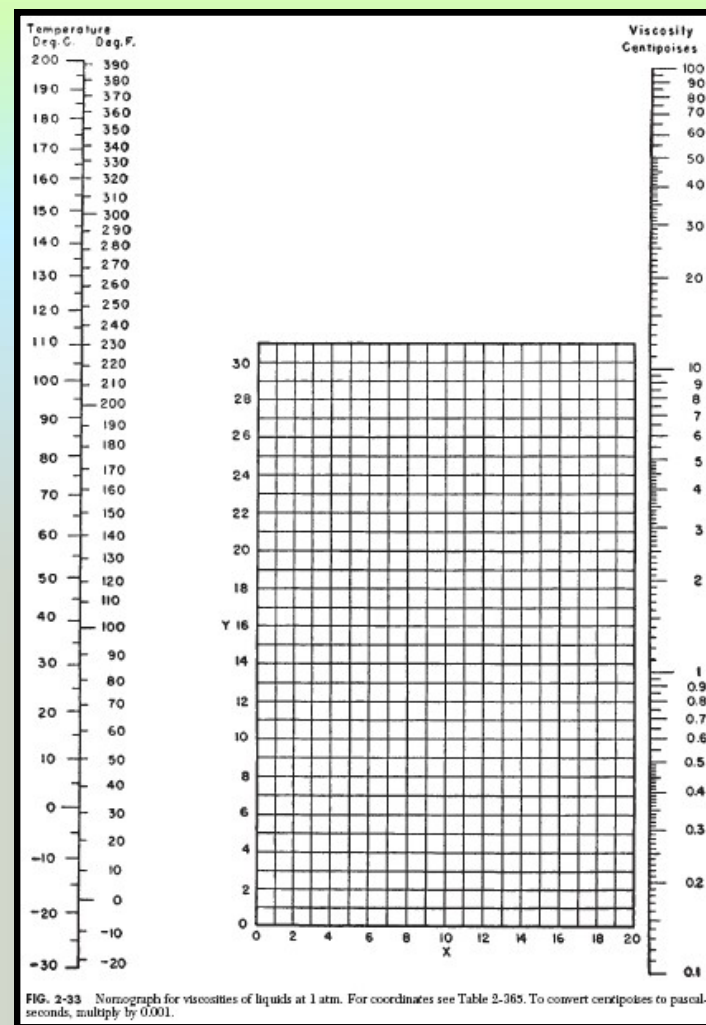


FIG. 2-32 Nomograph for determining (a) absolute viscosity of a gas as a function of temperature near ambient pressure and (b) relative viscosity of a gas compared with air. For coordinates see Table 2-364. To convert poises to pascal-seconds, multiply by 0.1. [From Beerman, Meas. Control, 154-157 (June 1982).]



**TABLE 2-365 Viscosities of Liquids: Coordinates for Use with**

Liquid	X	Y
Acetaldehyde	15.2	4.8
Acetic acid, 100%	12.1	14.2
Acetic acid, 70%	9.5	17.0
Acetic anhydride	12.7	12.8
Acetone, 100%	14.5	7.2
Acetone, 35%	7.9	15.0
Acetonitrile	14.4	7.4
Acrylic acid	12.3	13.9
Allyl alcohol	10.2	14.3
Allyl bromide	14.4	9.6
Allyl iodide	14.0	11.7
Ammonia, 100%	12.6	2.0
Ammonia, 26%	10.1	13.9
Amyl acetate	11.8	12.5
Amyl alcohol	7.5	18.4
Aniline	8.1	18.7
Anisole	12.3	13.5
Arsenic trichloride	13.9	14.5
Benzene	12.5	10.9
Brine, CaCl <sub>2</sub> , 25%	6.6	15.9
Brine, NaCl, 25%	10.2	16.6
Bromine	14.2	13.2
Bromotoluene	20.0	15.9
Butyl acetate	12.3	11.0
Butyl acrylate	11.5	12.6
Butyl alcohol	8.6	17.2
Butyric acid	12.1	15.3
Carbon dioxide	11.6	0.3
Carbon disulfide	16.1	7.5
Carbon tetrachloride	12.7	13.1
Chlorobenzene	12.3	12.4
Chloroform	14.4	10.2



**TABLE 2-366 Viscosity of Sucrose Solutions\***

Viscosity in centipoises

Temp., °C	Percentage sucrose by weight			Temp., °C	Percentage sucrose by weight		
	20	40	60		20	40	60
0	3.818	14.82		50	0.974	2.506	14.06
5	3.166	11.60		55	0.887	2.227	11.71
10	2.662	9.830	113.9	60	0.811	1.989	9.87
15	2.275	7.496	74.9	65	0.745	1.785	8.37
20	1.967	6.223	56.7	70	0.688	1.614	7.18
25	1.710	5.206	44.02	75	0.637	1.467	6.22
30	1.510	4.398	34.01	80	0.592	1.339	5.42
35	1.336	3.776	26.62	85	0.552	1.226	4.75
40	1.197	3.261	21.30	90		1.127	4.17
45	1.074	2.858	17.24	95		1.041	3.73

\**International Critical Tables*, vol. 5, p. 23. Bingham and Jackson, *Bur. Standards Bull.* 14 (1919): 59.



