

Chapter four

Kinetic Theory of Gases

4.1. Introduction

The kinetic theory of gases is concerned with the properties of idealized models of molecules. We will calculate the distribution of molecular speeds, the pressure of an ideal gas, and the rate of collision with a surface assuming point molecules. Then we will calculate the rates of molecular collisions and the mean free path assuming that the molecules are tiny hard spheres. These calculations will help us interpret the rates of chemical reactions. This simple model can also be used to calculate rates of mixing of gases by diffusion, the rate of conduction of heat, and viscosity. In general, matter is known to exist in one of the three states, Solid, liquid or gas. A solid may be defined as a body possessing definite volume and shape at a given temperature and pressure. Solids are orderly arrays of atoms, molecules, or ions having definite geometry depending upon the arrangements of these atoms, molecules or ions in a solid. Solids are relatively rigid. The constituents are held close together by strong attractive forces. A liquid, on the other hand, has a definite volume, but no definite shape. Molecules constituting a liquid are held by molecular forces which are not as strong as in solids. A gas has neither shape nor volume and the molecular forces of attractions are very much weaker. Gaseous state is the simplest state of matter and the laws and theories of gaseous behavior are more uniform and better understood.

Gases are conveniently classified into two types, namely, **ideal gases**, and **nonideal or real gases**. An ideal gas is one that obeys certain laws which will be dealt with shortly, while a real gas is one that obeys these laws at **low pressures** and relatively **high temperatures**. In ideal gases, the volume occupied by the molecules themselves is negligible as compared with the total volume at all pressures and temperatures. The intermolecular attraction is almost absent under all conditions. In case of real gases, both these factors are appreciable and the magnitude of each depends on the temperature and pressure of the gas and the nature of the gas.

Gases are one of the most pervasive aspects of our environment on the Earth. The steam formed in the air during a hot shower is a gas. The Helium used to fill a birthday balloon is a gas. The oxygen in the air is an essential gas for life.

Important Characteristics of Gases✓ **Gases are highly compressible**

An external force compresses the gas sample and decreases its volume, removing the external force allows the gas volume to increase.

✓ **Gases are thermally expandable**

When a gas sample is heated, its volume increases, and when it is cooled its volume decreases.

✓ **Gases have high viscosity**

Gases flow much easier than liquids or solids.

✓ **Most Gases have low densities**

Gas densities are on the order of grams per liter whereas liquids and solids are grams per cubic cm, 1000 times greater.

✓ **Gases are infinitely miscible**

Gases mix in any proportion such as in air, a mixture of many gases.

4.2. Kinetic Molecular Theory (KMT) of gases

The gas laws developed by Boyle, Charles, and Gay-Lussac are based upon empirical observations and describe the behavior of a gas in macroscopic terms, that is, in terms of properties that a person can directly observe and experience. An alternative approach to understanding the behavior of a gas is to begin with the atomic theory, which states that all substances are composed of a large number of very small particles (molecules or atoms). In principle, the observable properties of gas (pressure, volume, temperature) are the consequence of the actions of the molecules making up the gas.

The Kinetic Molecular Theory of Gases begins with five postulates that describe the behavior of molecules in a gas. These postulates are based upon some simple, basic scientific notions, but they also involve some simplifying assumptions. In reading a postulate, do two things. First, try to understand and appreciate the basic physical idea embodied in the postulate; this idea will ultimately be important in understanding the macroscopic properties of the gas in terms of the

behavior the microscopic molecules making up the gas. Second, identify possible weakness or flaws in the postulates. Inaccurate predictions by a theory derive from flawed postulates used in the derivation of the theory.

To better understand the molecular origins of the ideal gas law, $PV=nRT$, we need to understand the **Kinetic Molecular Theory of Gases (KMT)**. This model is used to describe the behavior of gases. More specifically, it is used to explain macroscopic properties of a gas, such as pressure and temperature, in terms of its microscopic components, such as atoms. Like the ideal gas law, this theory was developed in reference to ideal gases, although it can be applied reasonably well to real gases.

In order to apply the kinetic model of gases, five assumptions are made:

1. Gases are made up of particles with no defined volume but with a defined mass. In other words their volume is miniscule compared to the distance between themselves and other molecules.
2. Gas particles undergo no intermolecular attractions or repulsions. This assumption implies that the particles possess no potential energy and thus their total energy is simply equal to their kinetic energies.
3. Gas particles are in continuous, random motion.
4. Collisions between gas particles are completely elastic. In other words, there is no net loss or gain of kinetic energy when particles collide.
5. The average kinetic energy is the same for all gases at a given temperature, regardless of the identity of the gas. Furthermore, this kinetic energy is proportional to the absolute temperature of the gas.

Generally Particles in an ideal gas...

- ✓ have no volume.
- ✓ have elastic collisions.
- ✓ are in constant, random, straight-line motion.
- ✓ Don't attract or repel each other.

- ✓ have an avg. KE directly related to Kelvin temperature.

4.3. Ideal Gas Laws

An ideal gas is defined as one for which both the volume of molecules and forces between the molecules are so small that they have no effect on the behavior of the gas.

Ideal gas properties:

- ✓ Volume of gas molecules is negligible compared with gas volume
- ✓ Forces of attraction or repulsion between molecules or walls of container are zero
- ✓ No loss of internal energy due to collisions.

Since volume is directly proportional to Kelvin temperature, the volume of the gas should theoretically be zero at zero Kelvin. However gases liquefy or solidify before this low temperature reached. In fact low substances exist as a gas at a temperature near zero Kelvin. An ideal gas (a perfect gas) is a gas that obeys an ideal gas equation

Boyle's Law: As early as 1660, Robert Boyle performed a series of experiments in which he determined the effect of pressure on the volume of a given amount of air at a constant temperature. He found that the volume of any definite quantity of a gas at constant temperature varied inversely as the pressure of the gas. Mathematically,

$$V \propto \frac{1}{P} \text{ (Temperature and mass of the gas constant)}$$

$$PV = \text{constant} \dots \dots \dots (1)$$

Where V is the volume and P is the pressure of the gas. Thus if V_1 is the volume occupied by a given quantity of the gas at pressure P_1 , and V_2 is its volume when the pressure changes to P_2 , then at constant temperature it follows that:

$$P_1V_1 = P_2V_2 \text{ (Temperature and mass of the gas constant)}$$

OR

$$\frac{P_1}{P_2} = \frac{V_2}{V_1}$$

When the pressure of the gas is plotted against the volume in accordance with equation (1), we obtain curves (hyperbola) such as shown in Fig.1. These curves are known as **isotherms**. The upper curve corresponds to the higher temperature.

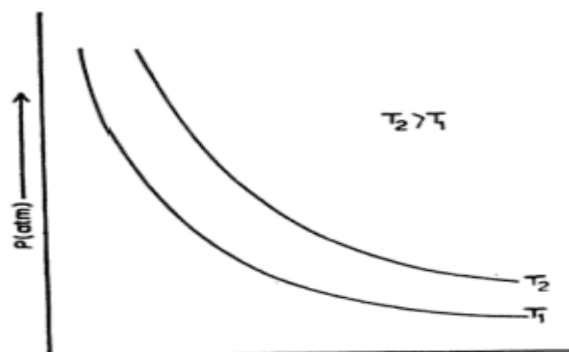


Figure 1. P -V plots for a given amount of gas at two temperatures.

2. Charles Law: Charles in 1787 studied the variation in volume of a gas with temperature at constant pressure and observed that the volume of a certain mass of the gas increases or decreases by $1/273.16$ of its value at 0°C . Mathematically it can be represented by:

$$\frac{V_2}{V_1} = \frac{T_2}{T_1}$$

This new temperature scale is known as the **Absolute or Kelvin scale of temperature** and is of fundamental importance in all sciences. This equation predicts that the volume of a definite quantity of a gas at constant pressure is directly proportional to the absolute temperature. Stated mathematically:

$$V \propto T \quad \text{or} \quad \frac{V}{T} = \text{constant} \dots \dots \dots (2)$$

According to equation (2) the volume of a gas should be a linear function of absolute temperature at constant pressure. Such a plot of V versus T at two pressures P_1 and P_2 ($P_2 > P_1$) is

shown in Figure 2. Each constant pressure line is called an **isobar**. For every -isobar the slope is greater lower the pressure.

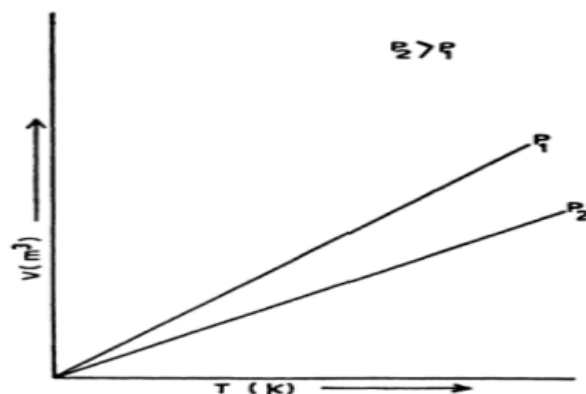


Figure 2: T-V plots for a given amount of gas at two pressures.

3. Avogadro Law: Avogadro in 1811 suggested that “equal volume of different gases at the same temperature and pressure contain equal number of molecules.” It will be recalled here that 1 mole of any substance contains the same number of molecules and that this number is known as the Avogadro’s number. It is represented by N and has a value 6.023×10^{23} . Hence we can write

$$V/n = \text{constant.}$$

$$\frac{V_1}{n_1} = \frac{V_2}{n_2}$$

4. Gay- Lussac Law: At constant volume, pressure and absolute temperature are directly related.

$$\frac{P_1}{T_1} = \frac{P_2}{T_2}$$

5. Combined ideal Gas Law: Boyle’s law, Charles law, Guy – Lussac law and Avogadro’s law can be combined to give a general relation between the volume, pressure, temperature and the number of moles of a gas. Equation (1) describes the variation of P with V at constant T and equation (2) represents the variation of V with T at constant P . i.e.

$$PV = \text{constant}$$

$$\frac{V}{T} = \text{constant}$$

On combining these equations, we get:

$$\frac{PV}{T} = \text{constant} \dots\dots\dots (3)$$

The combined equation (3) relating the variable P, V and T of an ideal gas is known as the equation of state. It is clear from equation (3) that the product PV divided by T is always constant for all specified states of the gas. Hence, if we know these values for any one state the constant can be computed. In the standard state (STP), the pressure is 1 atm and temperature 273.16 K. The volume occupied by a mole of an ideal gas under these conditions is 22.414 cm³ (22.414 litres). According to Avogadro's law this volume is the same for all ideal gases. If we consider at moles of an ideal gas at STP, then equation (3) becomes

$$\frac{PV}{T} = \frac{P_0V_0}{T_0} = nR \text{ OR } PV = nRT \dots\dots\dots (4)$$

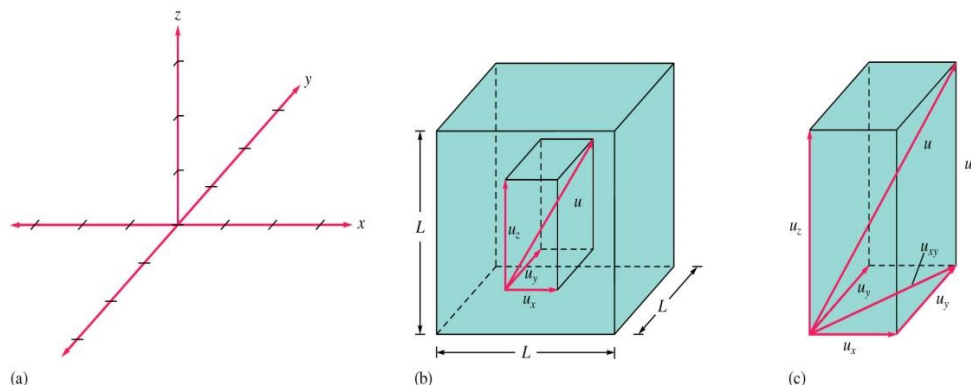
Where R is a universal gas constant. Equation (4) is known as the **ideal gas equation** and it connects directly the volume, temperature, pressure and the number of moles of a gas and permits all types of calculations as soon as the constant R is known.

Generally, an ideal gas is defined as one for which both the volume of molecules and forces between the molecules are so small that they have no effect on the behavior of the gas and their properties can be summarized as:

- ✓ Volume of gas molecules is negligible compared with gas volume
- ✓ Forces of attraction or repulsion between molecules or walls of container are zero
- ✓ No loss of internal energy due to collisions

4.4. Derivation of kinetic gas equation

Consider a collection of N molecules of an ideal gas in a container of volume V . Assume the container is a cube and its edges are length L . Look at the motion of the molecule in terms of its velocity components in three dimension and look at its momentum and the average force.



$$V^2 = V_x^2 + V_y^2 + V_z^2$$

- ✓ Where V is the velocity of the particle and V_x , V_y and V_z are components of the velocity along the three principal cartesian axes.

$$F = ma = m\left(\frac{\Delta v}{\Delta t}\right) = \Delta\left(\frac{mv}{\Delta t}\right)$$

$$\Delta mv_x = 2mv_x$$

- ✓ Recalling that the collision frequency $\Delta t = l/V_x$

$$F_x = Nm v_x \left(\frac{v_x}{l}\right) \text{ and similarly for } F_y \text{ and } F_z$$

$$\text{Thus: } F_{total} = \frac{Nmv_x^2}{l} + \frac{Nmv_y^2}{l} + \frac{Nmv_z^2}{l} = \frac{Nmv^2}{3l}$$

$$P = \frac{F_{tot}}{A_{tot}} = \frac{Nmv^2/3l}{l^2} = \frac{Nmv^2}{3l^3} = \frac{mNv^2}{3V}$$

✓ Since the number of particles in a given gas sample can be expressed as nN_A , where n is the number of moles and N_A is Avogadro's number.

$$P = nN_A \frac{mv^2}{3V} = \frac{2}{3} \left[\frac{nN_A \left(\frac{1}{2} mv^2 \right)}{V} \right] = \frac{2N}{3V} KE$$

This tells us that pressure:

- ✓ Is proportional to the number of molecules per unit volume (N/V)
- ✓ To the average translational kinetic energy of the molecules. The larger the velocity, more frequent collisions, greater change in momentum. $KE = N_A \left(\frac{1}{2} mv^2 \right)$

$$P = \frac{2}{3} \left[\frac{nKE}{V} \right] \text{ or } \frac{PV}{n} = \frac{2}{3} KE \propto T$$

$$\boxed{KE = \frac{3}{2} KT}$$

Two ideal gases at the same temperature will have the same average kinetic energy. If *temperature increases* at constant volume, the average kinetic energy of the gas molecules increases. Therefore, there are more collisions with the container walls and the **pressure increases**.

4.5. Barometric Formula

The **barometric formula**, sometimes called the *exponential atmosphere* or *isothermal atmosphere*, is a formula used to model how the pressure (or density) of the air changes with altitude.

The barometric formula can be derived fairly easily using the ideal gas law:

In this section we derive how the gas pressure P depends on the height over sea level h in the gravitational field of Earth.

If we take an arbitrary gas column with intersection area A and height h , then the weight of this column is given by:

$$F = mg = \rho gV = \rho ghA$$

Where ρ is the gas density. Then the gas pressure is expressed by the following formula:

$$P = \frac{F}{A} = \frac{\rho ghA}{A}$$

Now imagine such a column in the atmosphere and separate a thin layer of air with the height dh . It's clear that such a layer causes the pressure change by the value of

$$dP = -\rho gdh$$

We have put the minus sign because the pressure must decrease as the altitude increases.

Considering atmospheric air as an ideal gas, we can use the ideal gas law to express the density ρ through pressure P :

$$PV = \frac{m}{M}RT \Rightarrow P = \frac{m}{MV}RT = \frac{\rho}{M}RT$$

Here T is the absolute temperature, R is the universal gas constant equal to $8.314\text{JK}\cdot\text{mol}$, M is the molar mass, which is for air equal to 0.029kgmol . It follows from here that the density is given by the formula.

$$\rho = \frac{MP}{RT}$$

Putting this into the differential relation for dP gives:

$$dP = -\rho g dh = -\frac{MP}{RT} g dh \Rightarrow \frac{dP}{P} = -\frac{Mg}{RT} dh$$

We obtain a differential equation describing the gas pressure P as a function of the altitude h . integrating gives the equation

$$\int \frac{dP}{P} = -\int \frac{Mg}{RT} dh \Rightarrow \ln P = -\frac{Mg}{RT} h + C$$

Getting rid of the logarithms, we obtain the so-called barometric formula

$$P = C \exp\left(\frac{-Mg}{RT} h\right)$$

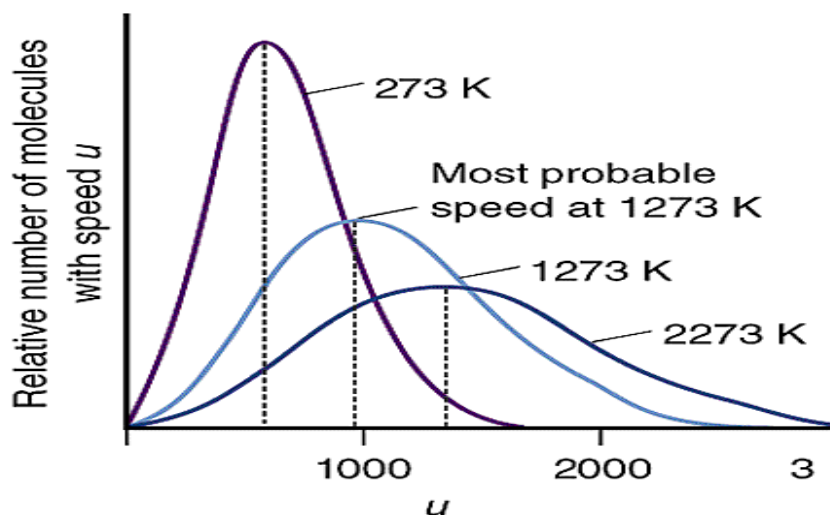
The constant of integration C can be determined from the initial condition $P(h = 0) = P_0$, where P_0 is the average sea level atmospheric pressure

Thus, dependency of the barometric pressure on the altitude is given by the formula

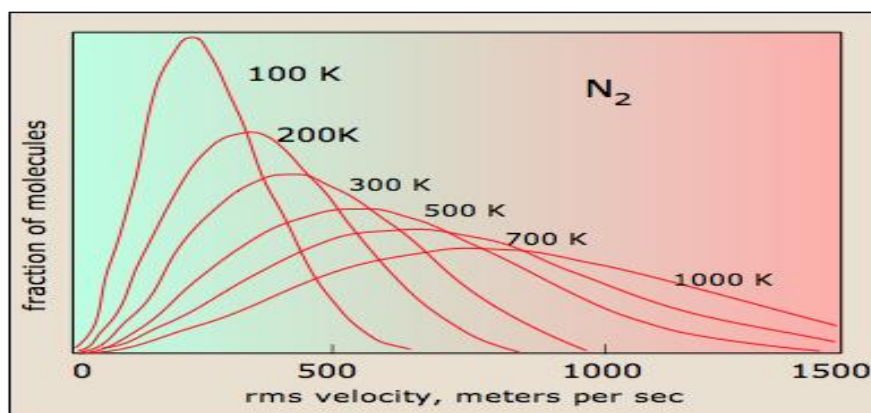
$$P = P_0 e^{\left(\frac{-Mg}{RT} h\right)}$$

4.6. Distribution of molecular velocities

The kinetic theory predicts the distribution function for the molecular speeds. Below we show the distribution of molecular speeds for N_2 gas at three temperatures.



Velocity distributions are dependent on the temperature and mass of the particles. As the temperature increases, the particles acquire more kinetic energy. On the plot of fraction of molecules versus velocity, we see that an increase in T^0 causes the Boltzmann plot to spread out, with the relative maximum shifting to the right. Larger molecular weights narrow the velocity distribution because all particles have the same kinetic energy at the same temperature.



By the equation: $-KE = \frac{1}{2}mv^2$ the fraction of particles with higher velocities will increase as the molecular weight decreases.

$$p(v) = 4\pi v^2 \left(\frac{m}{2\pi k_B T} \right) e^{-mv^2/2k_B T}$$

Where v = speed in m/s, m = mass of particle in kg

k_B = Boltzmann's constant = 1.38066×10^{-23} J/K T = temperature in K

$p(v) dv$ gives the fraction of molecules that have speeds between v and $v + \Delta v$. Velocity components of molecule are (v_x, v_y, v_z) and N molecules represented by N points in velocity space. Volume of space between v and $v + \Delta v$ is $\sim 4\pi v^2 \Delta v$. The minimum $p(v)$ moves to higher v as T° is raised. The speed at the maximum is the most probable speed

4.7. Different kinds of velocities

In explaining the distribution over speed the different speeds are: -

1. The most probable speed

- ✓ It is the speed at the maximum of $p(v)$ obtained by differentiating with respect to v and setting the result to give equal to zero.

$$\text{i.e. } \frac{dp(v)}{dv} = 0$$

$$\frac{dp(v)}{dv} = \left(\frac{m}{2\pi kT} \right)^{3/2} e^{-\frac{mv^2}{kT}} (8\pi v + 4\pi v^2 \left(\frac{mv}{kT} \right)) = 0$$

$$v = \left(\frac{2kT}{m} \right)^{1/2}$$

$$v_{mp} = \left(\frac{2kT}{m} \right)^{1/2}, \text{ but } k = \frac{R}{N_A}, R = kN_A$$

But $M = N_A m$

$$v_{mp} = \left(\frac{2kT}{m}\right)^{1/2} \left(\frac{N_A}{N_A}\right)^{1/2} = \left(\frac{2kTN_A}{N_A m}\right)^{1/2}$$

So
$$v_{mp} = \left(\frac{2RT}{M}\right)^{1/2} = \left(\frac{2kT}{m}\right)^{1/2}$$

5. **The mean speed** $\langle v \rangle$ is calculated as average of v using $p(v)$

$$\langle v \rangle = \int v p(v) dv = \left(\frac{8kT}{\pi m}\right)^{1/2} = \left(\frac{8RT}{\pi M}\right)^{1/2}$$

Where m = mass of single particle

M = molar mass

3. The Root mean square speed (V_{rms})

- ✓ It is the square root of $\langle v^2 \rangle$

$$v_{rms} = (\langle v^2 \rangle)^{1/2} = \left[\int_0^\infty v^2 p(v) dv \right]^{1/2} = \left(\frac{3kT}{m}\right)^{1/2} = \left(\frac{3RT}{M}\right)^{1/2}$$

From the above result of speeds all of them depends on temperature and mass of molecule and

$$V_{rms} > V_{ave} > V_{mp}$$

- ✓ In ratio $V_{rms} : \langle v \rangle : v_{mp} = 1 : 0.92 : 0.82$

Example

1. Calculate the V_{rms} , $\langle V \rangle$ and V_{mp} of hydrogen molecule at 0°C .
2. Find V_{rms} , $\langle V \rangle$ and V_{mp} for O_2 at 27°C .

4.8. Molecular Collisions

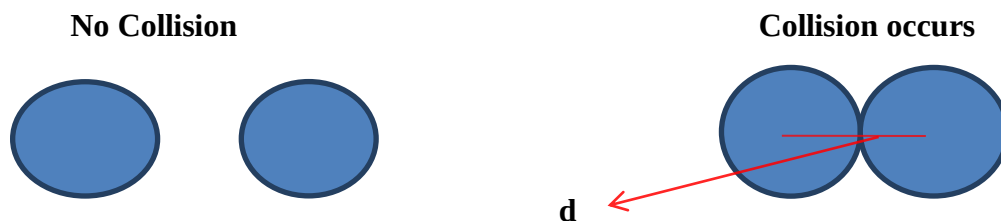
The collision of particles without internal structure is the simplest model for interacting molecules. A molecule is said to have undergone a “collision” if its interaction with another object results in a change in molecular direction. For a reaction to occur, molecules must collide. The collision frequency describes how many times a particular molecule collides with others per unit of time. In order for molecules to react, a physical chemist named Svante Arrhenius explained, the colliding molecules must possess enough KE to overcome the repulsive and bonding forces of the reactants. The minimum amount of energy required for a chemical reaction to occur is known as the activation energy (E_a).

The higher the (E_a) of a reaction, the smaller the amount of energetic collisions present and the slower the reaction. Energetic collisions are collisions between molecules with enough kinetic energy to cause the reaction to occur. Not all collisions are energetic collisions because they do not provide the necessary amount of (E_a), so not all collisions lead to reactions and product formation. In contrast, the lower the (E_a) of a reaction, the greater the amount of energetic collisions present, and the faster the reaction. Generally, a reaction cannot occur if the particles do not collide with the activation energy of the reaction.

There are two types of collision

1. Elastic collision: - is defined as one in which there is no loss of kinetic energy in the collision. When gases are left alone in a container do not seem to lose energy and do not spontaneously convert to the liquid.

2. In elastic collision: - is one in which part of the kinetic energy is changed to some other form of energy in the collision. Any macroscopic collision between objects will convert some of the kinetic energy into internal energy and other forms of energy. A pair of molecules will collide whenever the centers of the two molecules come within a distance d (the collision diameter) of one another.



Imagine one particle flying through stationary (frozen) particles. Within the $\sigma = \pi d^2$ area it will have collisions. The volume of the cylinder is given by:

$$V = L \times \sigma = \langle v \rangle \Delta t \sigma = \langle v \rangle \Delta t \pi d^2$$

To determine the collision frequency Z we have to consider the relative speed of the colliding particles.

$$\langle v \rangle = \left(\frac{8RT}{\pi M} \right)^{1/2} \quad \langle v \rangle_{rel} = \left(\frac{8RT}{\pi \mu_{12}} \right)^{1/2} \quad \mu_{12} = \frac{1}{M_1} + \frac{1}{M_2}$$

The reduced mass μ of two identical particles is $m/2$ and therefore:

$$\langle v \rangle_{rel} = (\langle v_1 \rangle^2 + \langle v_2 \rangle^2)^{1/2} = \sqrt{2} \langle v \rangle$$

To determine the collision frequency Z we determine the total number of molecules that have a collision in the time interval Δt . The number of centers N_d are the volume of the collision tube (with their relative velocities) multiplied with their density minus 1.

$$\langle v \rangle_{rel} = \sqrt{2} \langle v \rangle = \sqrt{2} \left(\frac{8kT}{\pi m} \right)^{1/2}$$

$$N_d = \left[\frac{N-1}{V} \right] \approx \frac{N}{V}$$

$$Z_1 = \frac{\langle v \rangle_{rel} \sigma \Delta t N_d}{\Delta t} = \sqrt{2} \langle v \rangle \sigma \frac{N}{V}$$

$$\text{With } \frac{N}{V} = \frac{P}{kT}$$

$$Z_1 = \sqrt{2} \langle v \rangle \sigma \frac{P}{kT}$$

The Collision Density

Collision density is the total rate of collisions per unit volume, and therefore multiply with the density N_d . The factor $\frac{1}{2}$ stems from the fact that only AB and not BA collisions are counted.

$$Z_{11} = \frac{1}{2} Z_1 \frac{N}{V} = \left(\frac{4kT}{\pi m} \right)^{1/2} \sigma \left[\frac{N}{V} \right]^{1/2}$$

The Mean Free Path (λ)

The mean free path - is the average distance traveled between successive collisions: velocity divided by collision frequency

$$\lambda = \frac{\langle v \rangle}{Z_1} \text{ With } Z_1 = \sqrt{2} \langle v \rangle \sigma \frac{P}{kT}$$

$$\lambda = \frac{\langle v \rangle}{\sqrt{2} \langle v \rangle \sigma \frac{P}{kT}} = \frac{1}{\sqrt{2}} \frac{kT}{\sigma P} = 0.707 \frac{kT}{\sigma P}$$

- The mean free path is inverse proportional with pressure.

Example

Diameter of Molecules, $D=2 \text{ \AA} = 2 \times 10^{-10} \text{ m}$, Collision Cross-section: $\sigma= 1 \times 10^{-19} \text{ m}^2$. calculate the mean free path at atmospheric pressure.

4.9. Collisions with a Surfaces or holes (Z_w)

Collision with the surface is calculated by using:

$$Z_w = \frac{N}{V} A \Delta t \int_0^{\infty} v_x \rho(v) dv$$

$$\int_0^{\infty} v_x \rho(v) dv = \sqrt{\frac{m}{2\pi kT}} \int_0^{\infty} v_x e^{-\frac{mv_x^2}{2kT}} dv_x \text{ with } \int_0^{\infty} x e^{-ax^2} dx = \frac{1}{2a}$$

$$= \sqrt{\frac{m}{2\pi kT}} \frac{2kT}{m}$$

$$= \sqrt{\frac{2kT}{\pi m}} = \frac{1}{4} \langle v \rangle$$

$$\frac{N}{V} = \frac{P}{kT}$$

$$Z_w = \frac{1}{4} \langle v \rangle \frac{N}{V} = \frac{P}{(2\pi kTm)^{1/2}}, \quad \sqrt{\frac{2kT}{\pi m}} = \frac{1}{4} \langle v \rangle$$

4.10. Transport Phenomena

In engineering, physics and chemistry, the study of **transport phenomena** concerns the exchange of mass, energy, and momentum between observed and studied systems. Transport of momentum, heat, and mass has an important role in various chemical, technological and natural processes. Identifying the transport properties of physical and chemical processes is crucial for

the optimization and scaling up of the processes especially in the chemical industries. In the Transport Phenomena research area, the transport properties in physical and chemical processes related to advanced materials processing, energy conversion and storage are studied. The main attention is given to understand the transport phenomena around solid-fluid interfaces.

The transport of mass, energy, and momentum can be affected by the presence of external sources:

- ✓ An odor dissipates more slowly (and may intensify) when the source of the odor remains present.
- ✓ The rate of cooling of a solid that is conducting heat depends on whether a heat source is applied.
- ✓ The gravitational force acting on a rain drop counteracts the resistance or drag imparted by the surrounding air.

An important principle in the study of transport phenomena is analogy between phenomena.

Diffusion

There are some notable similarities in equations for momentum, energy, and mass transfer which can all be transported by diffusion, as illustrated by the following examples:

- ✓ Mass: the spreading and dissipation of odors in air is an example of mass diffusion.
- ✓ Energy: the conduction of heat in a solid material is an example of heat diffusion.
- ✓ Momentum: the drag experienced by a rain drop as it falls in the atmosphere is an example of momentum diffusion (the rain drop loses momentum to the surrounding air through viscous stresses and decelerates).

The molecular transfer equations of Newton's law for fluid momentum, Fourier's law for heat, and Fick's law for mass are very similar. One can convert from one transfer coefficient to another in order to compare all three different transport phenomena.

Momentum transfer

In momentum transfer, the fluid is treated as a continuous distribution of matter. The study of momentum transfer or fluid mechanics can be divided into two branches: fluid statics (fluids at rest), and fluid dynamics (fluids in motion).

When a fluid is flowing in the x direction parallel to a solid surface, the fluid has x-directed momentum, and its concentration is $v_x\rho$. By random diffusion of molecules there is an exchange of molecules in the z direction. Hence the x-directed momentum has been transferred in the z-direction from the faster- to the slower-moving layer. The equation for momentum transport is Newton's Law of Viscosity written as follows:

$$\tau_{zx} = -\nu \frac{\partial \rho v_x}{\partial z}$$

where τ_{zx} is the flux of x-directed momentum in the z direction, ν is μ/ρ , the momentum diffusivity, z is the distance of transport or diffusion, ρ is the density, and μ is the viscosity. Newton's Law is the simplest relationship between the flux of momentum and the velocity gradient

Mass transfer

When a system contains two or more components whose concentration vary from point to point, there is a natural tendency for mass to be transferred, minimizing any concentration difference within the system. Mass Transfer in a system is governed by Fick's First Law: 'Diffusion flux from higher concentration to lower concentration is proportional to the gradient of the concentration of the substance and the diffusivity of the substance in the medium.' Mass transfer can take place due to different driving forces. Some of them are:

- ✓ Mass can be transferred by the action of a pressure gradient (pressure diffusion)
- ✓ Forced diffusion occurs because of the action of some external force
- ✓ Diffusion can be caused by temperature gradients (thermal diffusion)
- ✓ Diffusion can be caused by differences in chemical potential

This can be compared to Fick's Law of Diffusion:

$$J_{Ay} = -D_{AB} \frac{\partial C_A}{\partial y}$$

Where D is the diffusivity constant.

Energy transfer

All processes in engineering involve the transfer of energy. Some examples are the heating and cooling of process streams, phase changes, distillations, etc. The basic principle is the first law of thermodynamics which is expressed as follows for a static system:

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

The net flux of energy through a system equals the conductivity times the rate of change of temperature with respect to position.

For other systems that involve either turbulent flow, complex geometries or difficult boundary conditions another equation would be easier to use:

$$Q = h.A.\Delta T$$

Where A is the surface area, ΔT is the temperature driving force, Q is the heat flow per unit time, and h is the heat transfer coefficient.

Within heat transfer, two types of convection can occur.

Forced convection can occur in both laminar and turbulent flow. In the situation of laminar flow in circular tubes, several dimensionless numbers are used such as Nusselt number, Reynolds number, and Prandtl. The commonly used equation is:

$$Nu_a = \frac{h_a D}{k}$$

Natural or free convection is a function of Grashof and Prandtl numbers. The complexities of free convection heat transfer make it necessary to mainly use empirical relations from experimental data.

Heat transfer is analyzed in packed beds, reactors and heat exchangers.

The transport of matter in the absence of bulk flow is referred to as diffusion. The transport of heat from regions of high temperature to regions of lower temperature without convection is referred to as conduction and the transfer of momentum from a region of higher velocity to a region of lower velocity gives rise to the phenomenon of flow. In each case the rate of flow is proportional to the rate of change of some property with distance, a so-called gradient.