1- Units and Dimensions:-

Dimensions are our basic concepts measurement such as length, time, mass, temperature, and so on; *units* are the means of expressing the dimensions, such as feet or centimeters for length, and hours or seconds for time. By attaching units to all numbers that are fundamentally dimensionless, you get following very practical benefits:

a. diminished possibility of errors in your calculations,

- b. reduced intermediate calculations and time in problem solving.
- c. a logical approach to the problem than remembering a formula and substituting numbers

into the formula,

d. interpretation of the physical meaning of numbers you use.

In this book you will use two most commonly used systems of units:

- 1. SI, formally called Le Systeme Internationale d'Unites, and informally called S1 or more often (redundantly) the SI system of units.
- 2. or American Engineering system of units, not be confused with what is called the U.S. Conventional System (USCS) nor the English system of units.

The SI system has *certain advantages over the AE* system in fewer names are associated with the dimensions, and conversion one of units to another is easier. But in the United States the AE system has deep roots. Most modern computer programs i.e. (process simulators) allow use either or mixed sets of units. Dimensions and their respective units are classified as fundamental or derived:

- Fundamental (or basic) dimensions/units are those that can be measured independently and are sufficient to describe essential physical quantities.
- Derived dimensions/units are those that can be developed in terms of the fundamental dimensions/units.

Tables 1.1 and 1.2 list both basic, Derived and alternative units in the S1 and AE systems. Figure 1.1 illustrates the relation between the basic dimensions and some of the derived dimensions

Table 1.1 SI and CGS Units

Base Units		
Quantity	Units	Symbol
Length	meter (SI)	m
	centimeter (CGS)	cm
Mass	Kilogram (SI)	kg
	gram (CGS)	g
Moles	gram- mole	mol. or g- mole
Time	second	S
Temperature	kelvin	K
Electric current	ampere	А
Light intensity	candela	cd

Multiple Uni	t Preferences
tera (T) = 10^{12}	centi (c) = 10^{-2}
giga (G) = 10^9	mili (m) = 10^{-3}
mega (M) = 10^6	micro (μ) =10 ⁻⁶
kilo (k) = 10^3	nano (n) = 10^{-9}

Derived Units

Quantity	Unit	Symbol	Equivalent in Terms of Base Units
Volume	liter	L	0.001 m ³ 1000 cm ³
Force	newton (SI) dyne (CGS)	Ν	$\frac{1 \text{ kg} \cdot \text{m/s}^2}{1 \text{ g} \cdot \text{cm/s}^2}$
Pressure	pascal (SI)	Pa	1 N/m ²
Energy, work	joule (SI) erg (CGS) gram-calorie	J cal	$1 \text{ N} \cdot \text{m} = 1 \text{ kg} \cdot \text{m}^2/\text{s}^2$ $1 \text{ dyne} \cdot \text{cm} = 1 \text{ g} \cdot \text{cm}^2/\text{s}^2$ $4.184 \text{ J} = 4.184 \text{ kg} \cdot \text{m}^2/\text{s}^2$
Power	watt	w	$1 \text{ J/s} = 1 \text{ kg} \cdot \text{m}^2/\text{s}^3$

Physical Quantity	Name of Unit	Symbol
	Some Basic Units	
Length	foot	ft
Mass	pound (mass)	lbm
Time	second, minute, hour, day	s, min, h (hr), day
Temperature	degree Rankine or degree Fahrenheit	°R or °F
Molar amount	pound mole	lb mol
	Derived Units	
Force	pound (force)	lb _f
Energy	British thermal unit, foot pound (force)	Btu, (ft)(lbf)
Power	horsepower	hp
Density	pound (mass) per cubic foot	lbm/ft ³
Velocity	feet per second	ft/s
Acceleration	feet per second squared	ft/s ²
Pressure	pound (force) per square inch	lb ₄ /in. ² , psi
Heat capacity	Btu per pound (mass) per degree F	Btu/(lbm)(°F)

TABLE 1.2 American Engineering (AE) System Units Encountered in This Book



Figure 1.1 Relation between the basic dimensions (in boxes) and various derived dimensions (in ellipses).

Common Conv	version Factors
Length:-	Energy, Heat:-
1 ft = 12 in = 30.48 cm	$1Btu = 252 \text{ cal.} = 778 \text{ ft. Ib}_{f}$
<u>1 m =3.28 ft</u>	$1 J = 1 N.m = 10^7 erg$
<u>1 in =2.54 cm</u>	1 erg = 1 dyne. cm
1 mile = 5280 ft = 1.609 km	1 cal = 4.184 J
Volume:-	Power:-
1 Oil bbl (barrel) =42 gal	1 W= 1 J/sec
$1 \text{ ft}^3 = 7.48 \text{ gal} = 28.32 \text{ liters}$	$1 \text{ hp} = 550 \text{ ft. Ib}_{f}/\text{sec}$
$1 \text{ m}^3 = 35.31 \text{ ft}^3$	1 hp = 745.7 w = 0.7457 kw
1 us gal = 231 in^3	1 kw = 737.56 ft. Ibf /sec
$1 \text{ Liter} = 1000 \text{ cm}^3$	1 kw = 239 cal/sec
Mass:-	Density:-
1 Ib = 453.6 gm	$1 \text{ gm/cm}^3 = 62.43 \text{ Ib}_{\text{m}}/\text{ft}^3$
1 kg =2.2 Ib	$1 \text{ gm/cm}^3 = 1000 \text{ kg/m}^3$
$1 \text{ slug} = 32.17 \text{ Ib}_{\text{m}}$	$1 \text{ gm/cm}^3 = 8.34 \text{ Ib}_{\text{m}}/\text{ gal}$
1 ton(metric) = 1000 kg = 2204.6 Ib	Temperature:-
1 oz 28.34 gm	$T_{(K)} = T_{(^{\circ}C)} + 273$
Density:-	$T_{(R)} = T_{(^{\circ}F)} + 460$
$1 \text{gm/cm}^3 = 62.43 \text{ Ib}_{\text{m}}/\text{ft}^3$	1 degree $^{\circ}$ C =1.8 degree $^{\circ}$ F
$1 \text{gm/cm}^3 = 1000 \text{ kg/m}^3$	$T_{(^{\circ}F)} = 1.8 T_{(^{\circ}C)} + 32$
$1 \text{gm/cm}^3 = 8.34 \text{ Ib/ gal}$	$T_{(^{\circ}C)} = (T_{(^{\circ}F)} - 32)/1.8$
Force:-	$1 T_{(K)} = 1.8 T_{(R)}$
$1 \text{ dyen} = 1 \text{ gm.cm/sec}^2$	Viscisity:-
$1 \text{ N} = 1 \text{ kg.m/sec}^2 = 10^5 \text{ dyen}$	1poise =1 gm/cm. sec =100 cP
$1 \text{ Ib}_{\text{f}} = 4.448 \text{ N}$	$1 \text{ cP} = 2.42 \text{ Ib}_{\text{m}} / \text{ ft.hr}$
$1 \text{ Ib}_{\text{f}} = 32.17$	$1 \text{ cP} = 10^{-3} \text{ N.sec/m}^2$
Pressure:-	$1000 \text{ cP} = 1 \text{ N}. \text{ sec/m}^2 = 1 \text{ Pa.sec}$
1 atm. = 760 mmHg(torr)	
1 atm. = 29.92 in Hg	
1 atm. = 14.7 Ib_f / in^2 (psi)	
1 atm. = 2117 Ib_f/ft^2	
1 atm. = 33.93 ft water	
1 atm. = $1.013 \times 10^5 \text{ Pa} = 101.3 \text{ kPa}$	
1 Pa (Pascal) = 1 N/m^2	
$1 \text{ bar} = 10^5 \text{ Pa} = 100 \text{ kPa}$	

A system of units has the following components:-

- 1- Base units for mass, length, time, Temperature, electrical current and light intensity.
- 2- Derived units, obtained in one of two ways:
 - (a) By multiplying and dividing base or multiple units (Cm², ft/mn, kg.m/sec², ect.). Derived units of this type are referred to as compound units.
 - (b) As defined equivalents of compound units (e.g., 1 erg≈(1g.cm/s²), (1 Ibf ≈ Ibm.ft/s²).

*** The "system Internationale d"Unites" or SI for short, has gained widespread Acceptance. In the scientific and engineering community. Two of the base SI units- the ampere for Electrical current and candela for luminous intensity- will not concern us in this book. A third, the kelvin for temperature, will be discussed later. The others are the meter (m) For length, the kilogram (kg) for mass, and the second(s) for time.

*** The CGS system is almost identical to SI, the principal difference being centimeter (cm) are used instead of kilograms and meters as the base units of mass and length. The principal units of the CGS system are shown in table 2.3-1.

*** The base units of the **American engineering system** are the foot (ft) for length, the pound-mass (Ibm) for mass, and the second (s) for time. This system has two principal difficulties. The first is the occurrence of conversion factors (such as 1 ft/12 in), which, unlike those in the metric systems, are not multiples of 10; the second, which has to do with the unit of force is discussed in the next section.

<u>Symbols:-</u>

Any quantity can be expressed by a certain symbol which is more frequently used in calculation. A list of symbols of dimensions and of the most important secondary quantities are shown in the following table.

	Primary (Quantities	
Dimension	Symbol	Metric Units	English Units
Length	L	Cm or m	ft
Mass	М	gm or kg	Ib _m
Time	θ	sec	Sec, hr
Temperature	t or T	°C ,K	°F, R

	Secondary Quantities				
	Quantities	Symbol	Dimensional	Metric Units	English
			expression		Units
1	Area	А	L^2	m^2 , cm^2	ft^2
2	Volume	V	L^3	m ³ , liter	ft ³ , gal
3	Velocity	u	L/ 0	m/sec	ft./sec
4	Force	F	ML / θ^2	dyne, N	Ibf
5	Acceleration	а	L/θ^2	m/sec ²	ft/sec ²
6	Acceleration of gravity	g	L/θ^2	9.81 m/sec ²	32.17 ft/sec ²
7	Density	ρ	M/L^3	gm/cm^3 , Kg/m^3	Ibm/ft ³
8	Specific volume	V	L^3/M	m ³ /kg	ft ³ /Ib _m
9	Mass flow rate	ṁ	M/ θ	gm/sec, kg/hr	Ib _m /hr
10	Volumetric flow rate	V	L^{3}/θ	m ³ /hr, liter/sec	ft ³ /hr
11	Pressure	р	F/L^2	N/m ² (Pa),atm.	Ib _f /in ² (psi)
12	Viscosity	μ	Μ/Lθ	gm/ cm sec (poise)	Ib _m /ft sec
13	Heat	Q	Q, ML ² / θ^2	cal, J	Btu
14	Rate of heat transfer	q	Q/ θ	cal/sec, W	Btu/hr
15	Thermal conductivity	k	Q/ LT0	W/mk	Btu/hr ft F
16	Heat capacity	ср	Q/MT	cal/gm.°c	Btu / Ib_mF
				J /kg k	
17	Heat transfer coefficient	h	$Q/L^2T\theta$	W/m ² k sec	Btu/ft ² F hr
18	Work & energy	W, E	FL	J, erg	Ibf. ft
19	Power	Р	FL/θ	W	hp
20	Diffusivity	D _{AB}	L^{2}/θ	cm ² /sec	ft²/hr
21	Surface tension	б	F/L	dyne/cm	Ib _f /ft

Example: Conversion, Between Systems of Units

Example 1.1:-

Convert 23 $Ib_m.ft/min^2$ to its equivalent in kg.cm/s².

Solution:-

As before, begin by writing the dimensional equation, fill in the units of conversion factors (new/old) and then the numerical values of these factors, and then do the arithmetic. The result is

result is

$$\frac{23 \text{ lb}_{m} \cdot \text{ft}}{\text{min}^{2}} \frac{0.453593 \text{ kg}}{1 \text{ lb}_{m}} \frac{100 \text{ cm}}{3.281 \text{ ft}} \frac{1^{2} \text{ min}^{2}}{(60)^{2} \text{ s}^{2}} \quad \text{(Cancellation of units leaves kg} \cdot \text{cm/s}^{2}\text{)}$$
$$= \frac{(23)(0.453593)(100)}{(3.281)(3600)} \frac{\text{kg} \cdot \text{cm}}{\text{s}^{2}} = \boxed{0.088 \frac{\text{kg} \cdot \text{cm}}{\text{s}^{2}}}$$

Example 1.2:- Conversion of units

- (a) Convert 2 km to miles.
- (b) Convert 400 in.³/day to cm^3/min .

<u>Solution</u>:-

(a) One way to carry out the conversion is to look up a direct conversion factor, namely

1.61 km = 1 mile:

 $\frac{2 \text{ km}}{1.61 \text{ km}} = 1.24 \text{ mile}$ Another way is to use conversion factors you know $\frac{2 \text{ km}}{1 \text{ km}} \left| \frac{10^5 \text{ em}}{1 \text{ km}} \right| \frac{1 \text{ irr.}}{2.54 \text{ em}} \left| \frac{1 \text{ ff}}{12 \text{ irr.}} \right| \frac{1 \text{ mile}}{5280 \text{ fr.}} = 1.24 \text{ mile}$ (b) $\frac{400 \text{ in.}^3}{\text{day}} \left| \left(\frac{2.54 \text{ cm}}{1 \text{ in.}} \right)^3 \right| \frac{1 \text{ day}}{24 \text{ hr}} \left| \frac{1 \text{ hr}}{60 \text{ min}} \right| = 4.55 \frac{\text{cm}^3}{\text{min}}$

In part (b) note that not only are the numbers in the conversion of inches to centimeters raised to a power, but the units also are raised to the same power.

Example 1.3:- Nanotechnology

Nanosized materials have become the subject of intensive investigation in the last decade because of their potential use in semiconductors, drugs, protein detectors, and electron transport. Nanotechnology the generic term that refers to the synthesis and application of such small particles. An example of a semiconductor is ZnS with a particle diameter of 1.8 nanometers. Convert this value to (a) dm (decimeters) and (b) inches.

Solution

(a)
$$\frac{1.8 \text{ nm}}{|1.8 \text{ nm}|} \frac{10^{-9} \text{ m}}{|1.8 \text{ mm}|} \frac{10 \text{ dm}}{|1.8 \text{ m}|} = 1.8 \times 10^{-8} \text{ dm}$$

(b) $\frac{1.8 \text{ nm}}{|1.8 \text{ mm}|} \frac{10^{-9} \text{ m}}{|1.8 \text{ mm}|} \frac{39.37 \text{ in.}}{|1.8 \text{ mm}|} = 7.09 \times 10^{-8} \text{ in.}$

2- Force and Weight

According to Newton's second law of motion, force is proportional to the product of mass and acceleration (length/time²). Natural force units are, therefore, kg·m/s² (SI), g·cm/s² (CGS), and lb_m·ft/s² (American engineering). To avoid having to carry around these complex units in all calculations involving forces, *derived force units* have been defined in each system. In the metric systems, the derived force units (the **newton** in SI, the **dyne** in the CGS system) are defined to equal the natural units:

$$1 \text{ newton } (N) \equiv 1 \text{ kg} \cdot \text{m/s}^2$$
 (2.4-1)

$$1 \text{ dyne} \equiv 1 \text{ g} \cdot \text{cm/s}^2 \tag{2.4-2}$$

In the American engineering system, the derived force unit—called a **pound-force** (lb_f)—is defined as the product of a unit mass (1 lb_m) and the acceleration of gravity at sea level and 45° latitude, which is 32.174 ft/s²:

$$1 \, lb_{\rm f} = 32.174 \, lb_{\rm m} \cdot ft/s^2 \tag{2.4-3}$$

Equations 2.4-1 through 2.4-3 define conversion factors between natural and derived force units. For example, the force in newtons required to accelerate a mass of 4.00 kg at a rate of 9.00 m/s^2 is

$$F = \frac{4.00 \text{ kg} | 9.00 \text{ m} | 1 \text{ N}}{| s^2 | 1 \text{ kg} \cdot \text{m/s}^2} = 36.0 \text{ N}$$

The force in lbf required to accelerate a mass of 4.00 lbm at a rate of 9.00 ft/s² is

$$F = \frac{4.00 \text{ lb}_{\text{m}}}{|\mathbf{s}^2|} \frac{9.00 \text{ ft}}{32.174 \text{ lb}_{\text{m}} \cdot \text{ft/s}^2} = 1.12 \text{ lb}_{\text{f}}$$

Factors needed to convert from one force unit to another are summarized in the table on the inside front cover. The symbol g_c is sometimes used to denote the conversion factor from natural to derived force units: for example,

$$g_c = \frac{1 \text{ kg} \cdot \text{m/s}^2}{1 \text{ N}} = \frac{32.174 \text{ lb}_{\text{m}} \cdot \text{ft/s}^2}{1 \text{ lb}_{\text{ft}}}$$

We will not use this symbol in the text, but if you should encounter it elsewhere remember that it is simply a conversion factor (not to be confused with gravitational acceleration, which is usually denoted by g).

The weight of an object is the force exerted on the object by gravitational attraction. Suppose that an object of mass m is subjected to a gravitational force W (W is by definition the weight of the object) and that if this object were falling freely its acceleration would be g. The weight, mass, and free-fall acceleration of the object are related by Equation 2.4-4:

$$W = mg \tag{2.4-4}$$

The gravitational acceleration (g) varies directly with the mass of the attracting body (the earth, in most problems you will confront) and inversely with the square of the distance between the centers of mass of the attracting body and the object being attracted. The value of g at sea level

and 45° latitude is given below in each system of units:

$$g = 9.8066 \text{ m/s}^2$$

= 980.66 cm/s²
= 32.174 ft/s² (2.4-5)

The acceleration of gravity does not vary much with position on the earth's surface and (within moderate limits) altitude, and the values in Equation 2.4-5 may accordingly be used for most conversions between mass and weight.

Example1.4:- Weight and Mass

Water has a density of 62.4 Ib_m/ft^3 . How much does 2 ft³ of water weigh (1) at sea level and 45° latitude and (2) in Denver, Colorado, where the altitude is 5374 ft and gravitational acceleration is 32.139 ft/s²?

<u>Solution:</u>

The mass of the water is

$$M = \left(62.4 \ \frac{\text{lb}_{\text{m}}}{\text{ft}^3}\right) (2 \ \text{ft}^3) = 124.8 \ \text{lb}_{\text{m}}$$

The weight of the water is

$$W = (124.8 \text{ lb}_{m})g\left(\frac{\text{ft}}{\text{s}^{2}}\right)\left(\frac{1 \text{ lb}_{f}}{32.174 \text{ lb}_{m} \cdot \text{ft/s}^{2}}\right)$$

- 1. At sea level, g = 32.174 ft/s², so that W = 124.8 lb_f.
- 2. In Denver, g = 32.139 ft/s², and W = 124.7 lb_f.

As this example illustrates, the error incurred by assuming that g = 32.174 ft/s² is normally quite small as long as you remain on the earth's surface. In a satellite or on another planet it would be a different story.

3- Newten's Law Conversion Factor (gc):-

In the AE system the conversion of tems involving pound mass and pound force deserve special attention. Let us start the discussion with Newton's Law:

$$\mathbf{F} = \mathbf{C} \ \mathbf{m} \ \mathbf{a} \tag{1.1}$$

Where:- F =force, m =mass, a =acceleration

C = a constant whose numerical value and units depend on those Selected for F. m, and a.

cgs system	American system	SI system
F=1 dyne	F=1 Ibf	F=1 N
m= 1 gm	m= 1 Ibm	m= 1 kg
$a = 1 \text{ cm/sec}^2$	$a = 1 \text{ ft/sec}^2$	$a = 1 \text{ m/sec}^2$
$C = 1 \frac{dyne \ sec^2}{gm. \ cm}$	$C = \frac{1}{32.174} \frac{Ib_f sec^2}{Ib_m . ft}$	$C = 1 \frac{N \sec^2}{kg m}$

The inverse of the conversion factor with the numerical value 32.174 included is given the special symbol (gc).

The term $g_c = \frac{1}{c}$ is selected as a conversion factor to convert mass units to force and vice versa with the following values:-

cgs system	American system	SI system
$g_c = 1 \; \frac{gm.cm}{dyne.sec^2}$	$g_c = 32.174 \ \frac{Ib_m . ft}{Ib_f . sec^2}$	$g_c = 1 \frac{kg.m}{N sec^2}$

That you will see included in equations in some texts to remind you that the numerical value of conversion factor is not a unity. To avoid confusion, we will not place gc in the equations in this book because we will be using both SI and AE units.

You will discover that the use of gc is essential in the AE system when need a conversion factor to adjust units when both Ibm and Ibf are involved in a calculation, or when Ibf has to be transformed to Ibm in a unit such as psia (lb_f/in^2).

In summary, you can see that the AE system has convenience that the numerical value of a pound mass is also that of a pound force if the numerical value of the ratio g/gc equal to 1, as it is approximately most cases. No one gets confused by the fact that a person who 6 feet tall has only two In this book, we will not subscript the symbol lb with m (for mass) or f (for force) unless it becomes essential to do so to avoid confusion.

We will always mean by the unit Ib without a subscript quantity pound mass. But never forget that the pound (mass) and pound (force) are not the same units in the AE system even though we speak of pounds to express force, weight, or mass.

Example:-1.4 A conversion Involving Both Ib_m and Ib_f

What is the potential energy in (ft) (Ib_f) of a 100 Ib_m drum hanging 10 ft above the surface of the earth with reference to the surface of the earth?

<u>Solution:-</u>

The first thing to do is read the problem carefully. What are the unknown quantities? The potential (*PE*) is unknown. What are the known quantities? The mass and the height the drum are known. How are they related? You have to look up the relation unless you it from physics: **Potential energy = PE = mg h**

Assume that the 100 Ib means 100 Ib mass;

 $g = acceleration of gravity = 32.2 \text{ ft /sec}^2$

Figure 31.4 is a sketch of system.





Now substitute the numerical values of the variables into the equation and perform the necessary unit conversions.

$$P = \frac{100 \text{ lb}_{\text{m}}}{|s^2|} \left| \frac{32.2 \text{ ft}}{s^2} \right| \frac{10 \text{ ft}}{|s^2|} \left| \frac{(s^2)(\text{lb}_{\text{f}})}{32.174(\text{ft})(\text{lb}_{\text{m}})} \right| = 1000 \text{ (ft)}(\text{lb}_{\text{f}})$$

Notice that in the ratio of 32.2 ft/sec^2 divided by $32.174 [(\text{ft})(\text{lb}_m)]/[(\text{s}^2)(1\text{b}_f)]$, the numerical, values are almost equal. Many engineers would solve the problem by saying that 100 lb x 10 ft =1000 (ft)(lb) without realizing that, in effect, they are canceling out the numbers in the g/gc ratio, and that the Ib in the solution means Ib_f.

<u>Example:-1.5</u> Conversion of Units Associated with Biological Materials

In biological systems, enzymes are used to accelerate the rates of certain biological reactions. Glucoamylase is an enzyme that aids in the conversion of starch to glucose (a sugar that cells use for energy). Experiments show that $1\mu g$ mol of glucoamylase in a 4% starch solution results in a production rate of glucose of 0.6 μg mol. /(mL)(min). Determine production rate of glucose for this system in the units of Ib mol. / (ft³) (day).

<u>Solution:-</u> Basis: 1 min

Solution

Basis: 1 min $\frac{0.6 \ \mu \text{g mol}}{(\text{mL})(\text{min})} \left| \frac{1 \ \text{g mol}}{10^6 \ \mu \text{g mol}} \right| \frac{1 \ \text{lb mol}}{454 \ \text{g mol}} \left| \frac{1000 \ \text{mL}}{1 \ \text{L}} \right| \frac{1 \ \text{L}}{3.531 \ \times \ 10^{-2} \ \text{ft}^3} \left| \frac{60 \ \text{min}}{\text{hr}} \right| \frac{24 \ \text{hr}}{\text{day}}$ $= 0.0539 \frac{\text{lb mol}}{(\text{ft}^3)(\text{day})}$

4- Dimensional Consistency (Homogeneity) and Conversion of Units:-

The basic principle of dimensional consistency states that any equation consists of different physical quantities must be dimensionally consistent.

i.e. the units of both sides of the equation must be equivalent.

This concept can be used to determine the units of any unknown term in the equation and also to check the accuracy of the equation

In general, the fallowing steps can be used to convert the units of any quantity from one system to the anther or to calculate any quantity according to a specific equation by certain units:

- 1- Write the desired units of the quantity on the left side of the equation.
- 2- Write the units of the given data on the right side of the equation.
- 3- Balance the units of the both sides of the equation by multiplying the right side by the appropriate conversion factor.
- 4- Insert the numerical values of the conversion factors used to balance the equation to get the final answer.

Example 1:-

Van der Waals's equation, represents real gaseous behavior:-

$$\left(p+\frac{n^2a}{V^2}\right)(V-nb)=nRT$$

Where (a) and (b) are Van der Waals's constants.

If the unit of pressure in (atm.) and volume is given (cm³), what the units of (a) and (b)?

Solution:-

The unit of the term $\frac{n^2 a}{V^2}$ must be the same of (**p**).

Hence, the unit of (a) is $[atm.(\frac{Cm^3}{mol})^2]$

Similarly, the unit of (b) is $\left(\frac{Cm^3}{mol}\right)$

Example 2:-

The rate of heat transfer by convection is given by the following relation:-

 $q = h A \Delta T$

Where q = rate of heat transfer (J/s)

 $A = area (m^2)$

h= heat transfer coefficient

What are the units of h?

<u>Solution:</u>

$$h = \frac{q}{A \ \Delta T}$$

Hence, the units of

$$h = \frac{J}{s m^2 k}$$
 or $\frac{W}{m^2 K}$

5- Dimensionless Numbers:-

Most of the chemical engineering relations are formulated by putting the variables in dimensionless group's numbers. Each numbers was suggested theoretically or based an experiment by grouping the involved variables and put them together in the form that have no net units and known by the name of the investigator that suggest its equation.

One example is the Reynolds number (Re) which arise by Osborn Reynolds in 1883 in the field of fluid machines. He showed that the type of flow of a flawing fluid through a pipe depends on:-

- 1- Fluid velocity (u)
- 2- Fluid density (ρ)
- 3- Fluid viscosity (μ) and
- 4- The pipe diameter (d).

He suggests the fallowing dimensionless number as an indication for the type of flow:

Reynolds number
$$= \frac{\rho u D}{\mu} = N_{RE}$$

When	Re < 2100,	the flow is laminar and the fluid flow in
		Smooth stream lines.
For	Re > 3000,	the flow is turbulent so that internal agitation
		Or eddy currents takes place.
For	2100 < Re < 3000,	the flow is in transition region between
		Stream line and turbulent flow conditions.
C		$Cp \mu$ D

Similarly, Prenatal number $(p_r) = \frac{cp \mu}{k}$ and Nusselt number $(N_U) = \frac{h d}{k}$

The general relationship for heat transfer to or from a moving fluid through a pipe is of the form: $N_U = C (R_E)^a (P_r)^b$

Where a,b and c are constant:-

On the other hand, the general relationship for mass transfer is of the form:

$$Sh = C \ (R_E)^a (S_C)^b$$

Where:- (Sh) is Sherwood number (Sh) = $\frac{k_c d}{D_{AB}}$ and

(S_c) is Schmidt number (S_c) = $\frac{\mu}{\rho D_{AB}}$

Note:- kc is the mass transfer coefficient which is the term similar to the heat transfer Coefficient (h).

Example 3:-

What are the units of the constant k in the following equation?

$$\Delta p = \frac{k f l \rho u^2}{d}$$

Where f: friction factor (dimension less), Δp : pressure drop, and l: length *Solution:*-

$$k = \frac{\Delta p \, d}{f \, l \, \rho \, u^2} = \frac{\frac{F}{L^2} * L}{L * \frac{M}{L^3} * \frac{L^2}{\theta^2}} * g_c \left[\frac{M \, L}{F \, \theta^2}\right]$$

:. The constant (k) is dimensionless

Example 4:-

Check the dimensional consistency of the following equation:-

$$q = \frac{k A \Delta T}{r}$$

Where k: thermal conductivity, and x: distance

Solution:-

$$left \ side = q = \frac{Q}{\theta}$$

$$Right \ side = \frac{k \ A \ \Delta T}{x} = \frac{\frac{Q}{L \ T \ \theta} * \ L^{2} * \ T}{L} = \frac{Q}{\theta}$$

:. The equation is dimensionally consistent.

chapter2: -

***Basic Definitions and conventions:-

In this section some of definition and concepts important quantities by detail and which are of importance in chemical engineering calculation and practice.

Density, Specific volume and specific gravity:-

<u>1-</u> <u>**Density:-**</u> is the ratio of mass per unit volume, as example, kg/m³ or Ib/ft³.

$$\rho = density = \frac{mass}{volume} = \frac{m}{V}$$

Density has both a numerical value and units. To determine the density a substance. You find both volume and mass.

Densities for liquids and solids do not change significantly at ordinary conditions with pressure, but they do change with temperature, as shown in Figure 1. Usually we will ignore the effect, of temperature on liquid density.

On the other hand, density of mixture varies considerably with composition as shown in the figures for ethanol-water mixture and for sodium chloride solution.



*Figure 2.1 Densities of liquid H*₂*O and NH*₃ *as a function of temperature.*

<u>Density Measurement:-</u>

Hydrometer and pycnometer are the most important instruments which are commonly used for density measurement of liquids.

Density of gas can be estimated theoretically under any condition from ideal or real laws.

Density of solids can be determined directly from the measurement of mass and volume.



Figure 2.2 Density of a mixture of ethyl alcohol and water as a function of composition.



Fig. 2.3 Changes in density of aqueous solutions with changes in concentration at 20°C.

<u>2-</u> <u>Specific volume</u>:

is the inverse of density, such as cm^3/g , m^3/kg , $m^3/mole$ or ft^3/lb . this meaning the ratio of volume per unit mass or unit mole with the units. This term widely used rather than density for gases and vapours. For a compound.

$$\rho = \text{density} = \frac{\text{mass}}{\text{volume}} = \frac{m}{V}$$

 $\hat{V} = \text{specific volume} = \frac{\text{volume}}{\text{mass}} = \frac{V}{m}$

So that given the density of the compound you can calculate the volume a given mass. For example, given that the density of n-propyl alcohol is 0.804 g/cm^3 , what would the volume of 90.0 g of alcohol? The calculation is

$$\frac{90.0 g}{0.804 g} = 112 \text{ cm}^3$$

Some quantities related to density are molar density $(\frac{\rho}{Mw})$ and molar volume $(\frac{Mw}{\rho})$. By analogy, in a packed bed of solid particles containing void spaces, the bulk density is

 $\rho_B = \text{bulk density} = \frac{\text{total mass of solids}}{\text{total empty bed volume}}$

A homogeneous mixture of two or more components, whether solid, liquid, or gaseous, is called a **solution**. Solutions have variable composition while pure substances do not. That the relative amounts of the various components in a solution can vary. Thus, air, salt water, and 16-carat gold each are solutions. For some solutions, to calculate the density of the solution, you can make a linear combination of the individual components by adding the respective masses and volumes, and then dividing:

$$V = \sum_{i=1}^{n} V_i \quad \text{where } n = \text{number of components}$$
$$m = \sum_{i=1}^{n} m_i$$
$$\rho_{\text{solution}} = \frac{m}{V}$$

<u>3-</u> <u>SpeicificGravity(spg):-</u>

Specific volume is the ratio between the densities of the substance (ρ_A) to the density of reference substance (ρ_{ref}) at a specific condition,

Hence it is a dimensionless ratio. $(spg)_A = \frac{\rho_A}{\rho_{ref}}$

The reference substance for liquids and solids is normally water at 4°c. The specific gravity of gases frequently is referred to air either at the same conditions of the gas or at the standard conditions. Which has the following density:

sp.gr. of
$$A$$
 = specific gravity of $A = \frac{(g/cm^3)_A}{(g/cm^3)_{ref}} = \frac{(kg/m^3)_A}{(kg/m^3)_{ref}} = \frac{(lb/ft^3)_A}{(lb/ft^3)_{ref}}$
 $\rho_{water} at 4^{\circ}c$ = 1 g/cm³ = 1000 kg/m³ = 62.43 Ib_m/ft³ 8.34 Ib_m/gal

Note:

When referring to specific gravity, the data should be accompanied by both the temperature of the substance of interest and the temperature at which the reference density is measured. Thus, for solids and liquids the notation

sp.gr. =
$$0.73 \frac{20^\circ}{4^\circ}$$

Means the specific gravity when the substance solution is at 20° c and the substance reference (water) is at 4° c is 0.73.

EXAMPLE 2.4 Calculation of Density Given the Specific Gravity

If a 70% (by weight) solution of glycerol has a specific gravity of 1.184 at 15°C, what is the density of the solution in (a) g/cm^3 ? (b) lb_m/ft^3 ? and (c) kg/m³?

Solution

Use the specific gravity to get density via a reference substance.

No temperatures are cited for the reference compound (presumed to be water), hence for simplicity we assume that the temperatures of the water is 4°C, and that water has a density of $1.00 \times 10^3 \text{ kg/m}^3$ (1.00 g/cm³). The answers are:

- (a) 1.184 g solution/cm³ (calculated in your head)
- (b) $(1.184 \text{ lb glycerol/ft}^3)/(1 \text{ lb water/ft}^3) \times (62.4 \text{ lb water/ft}^3) = 73.9 \text{ lb solution/ft}^3$
- (c) 1.184×10^3 kg solution/m³ (calculated in your head).

*******Partial Scales of specific Gravity:-

Many scales are used in general practice. The following scales are widely used in various

Industries.

1- API Scale (*API):-

The degree of American Petroleum Institute (°API) is usually used in petroleum industry for evolution of petroleum product.

°API =
$$\frac{141.5}{\text{sp.gr.} \frac{60^{\circ}\text{F}}{60^{\circ}\text{F}}}$$
 - 131.5 (API gravity) (2.1)

or

$$sp.gr.\frac{60^{\circ}}{60^{\circ}} = \frac{141.5}{^{\circ}API + 131.5}$$
(2.2)

2- Degree Baume (*Be):-

This scale is widely used to express the specific gravity of solutions specifically sulfuric acid solutions Two Baume scales are in common use one for liquids lighter and the other for liquids heavier than water.

$${}^{\circ}Be_{h} = 145 - \frac{145}{spg}$$
 (For liquids heavier than water).
$${}^{\circ}Be_{l} = \frac{140}{spg} - 130$$
 (For liquids lighter than water).

3- Degree Twadell (*Tw):-

This scale is used only for liquids heavier than water. It has the advantage of a Simple relationship to specific gravities.

$$^{\circ}\mathrm{T}_{\mathrm{W}}=200(spg-1)$$

Tabulated values of °API, °Be and °Tw for different specific gravities within the range of 0.600 - 2.00 are shown in the following table.

4- Degree Brix (*Bx):-

This scale is widely used in sugar industry. It is graduated arbitrarily so that $1 \text{ }^{\circ}Bx = 1 \text{ wt\%}$ sugar.

$$^{\circ}BX_{l} = \frac{400}{spg} - 400$$
 (For liquids lighter than water).
$$^{\circ}BX_{h} = 400 - \frac{400}{spg}$$
 (For liquids heavier than water). In general, the

density or specific gravity may be used as an index to the concentration of solutions. This method is useful only when there is a large difference between the densities of the solutions and that of the pure solvent. In several industries the scales of specific gravity are the universally accepted means of indicating the concentration. Sulfuric acid, for example is marketed almost entirely on the basis of its °Be specifications.

The following tables shows the relations of °Be &°Tw with concentrations of sulfuric acid, caustic soda and sodium carbonate solutions.

Comparison between Brix scale with Baume and Twadell scales for different sugar solutions are shown below:

•Bx (wt% sugar)	spg	•Be	• <i>Tw</i>
33	1.090	12	18
41.3	1.115	15	23
55.2	1.160	20	32

<u>Example 13:</u>

Calculate the mass in kg of 200 liter of 50 °Tw salt solution. *Solution:*

°Tw= 200 (spg-1) $rac{spg}{spg} = \frac{{}^{\circ}T_W}{200} + 1$

$$spg = \frac{50}{200} + 1 = 1.25$$

$$\rho_{sol.} = spg * \rho_{water} = 1.25 * \frac{1 kg}{1 liter} = 1.25 \frac{kg}{liter}$$

*Mass of*_{sol.} =
$$\rho_{Sol.} * V = 1.25 \frac{kg}{liter} * 200 liter = 250 kg$$

Example 14:

Calculate the volume in bbl accupied by 1000 Ib of 25 °API gas oil.

Solution:
$$spg = \frac{141.5}{^{\circ}API + 131.5} = \frac{141.5}{156.5} = 0.9042$$

$$\rho_{gas \ oil} = spg * \rho_{water} = 0.9042 * 8.34 \frac{lb}{gal} = 7.54 \frac{lb}{gal}$$

$$\rho = \frac{M}{V} \qquad \therefore V = \frac{M}{\rho} = \frac{1000 \ lb}{7.54 \ \frac{lb}{gal}} = 132.6 \ gal$$

$$Volume \ of_{gas \ oil} = 132.6 \ gal * \frac{bbl}{42 \ gal} = 3.16 \ bbl$$

Example 15:

Calculate the mass in Ib of 250 gal of 27 °Be nitric acid solution. (Heavier than water)

Solution:-

$${}^{\circ}Be = 145 - \frac{145}{spg}$$

$$spg = \frac{145}{145 + {}^{\circ}Be} = \frac{145}{145 - 27} = 1.2288$$

$$\rho_{sol.} = spg * \rho_{water} = 1.2288 * 8.34 \frac{lb}{gal} = 10.428 \frac{lb}{gal}$$

$$Mass = \rho_{sol.} * V = 10.248 \frac{lb}{gal} * 250 \ gal = 2562 \ lb$$

Chapter3: - <u>The Mole unit</u>

The word mole appears to have introduced by William Ostwald in 1896, who took it from the Latin word moles meaning "heap" or "pile." i.e. the mole can be considered as a large heap of particles.

A more precise definition was out by the "International Committee on Weights and Measures" in 1969. Which defined the mole (symbol mol in the SI system) as the amount of a substance that contains number of elementary entities (i.e. atoms, molecules, ions or other particles) equal to that in 0.012 kg of carbon12 (6.023×10^{23}).

In the SI system a mol of a substance consisting of 6.022×10^{23} molecules. This number is known as (Avogadro's Number). However, it should be remembered that the term gram mole is used in cgs system which equal to mol in SI system.

There are other molar units which have the same conversion factors of the mass units as follow:

1 lb mole = 453.6 mol 1 Kg mol or kmol = 1000 mol

The term gram- atom is defined as the quantity of element that consists of 6.022×10^{23} atoms. This term is widely used to relate the quantities of elements within the molecule of compound as given by the molecular formula.

The following relation very important and used to convert the number of moles to mass and the mass to moles.

$$number of moles = \frac{Mass of the substance}{Molecular weight}$$
$$number of g.atoms = \frac{Mass of element in gm}{atomic weight}$$

Thus, the calculations you carry out are

the
$$g mol = \frac{Mass in g}{Molecular weight}$$

the Ib mol = $\frac{Mass in Ib}{Molecular weight}$

and

mass in
$$g = (MW)(g mol)$$

mass in $Ib = (MW)(Ib mol)$

For example

$$\frac{100.0 \text{ g H}_2\text{O}}{\frac{1 \text{ g mol H}_2\text{O}}{18.0 \text{ g H}_2\text{O}}} = 5.56 \text{ g mol H}_2\text{O}$$

$$\frac{6.0 \text{ lb mol O}_2}{\frac{1 \text{ g mol H}_2\text{O}}{1 \text{ lb mol O}_2}} = 192 \text{ lb O}_2$$

It is important to remember that atomic weight is an arbitrarily scale of the relative mass of atoms of the elements so that it represents the mass of an atom of the element referred to 12 as the mass of carbon isotope atom 12 C.

<u>Molecular weights (Mwt):</u> - represents the sum of the atomic weight of the elements as given by the molecular formula of the substance. The units of Mwt are (gm/mol, Ib/Ib mol or kg/kmol).

Example 2.1 Use of Molecular Weights to Convert Mass to Moles

If a bucket holds 2.00 Ib of NaOH. How many

- (a) Pound moles of NaOH does it contain?
- (b) moles of NaOH does it contain?

Solution

You want to convert pounds to pound moles, and then convert respective values to the SI units. Look up the molecular weight of NaOH. or calculate it from the atomic weights. It is 40.0.

(a)
$$\frac{2.00 \text{ lb NaOH}}{40.0 \text{ lb NaOH}} = 0.050 \text{ lb mol NaOH}$$

(b₁) $\frac{2.00 \text{ lb NaOH}}{40.0 \text{ lb NaOH}} \left| \frac{1 \text{ lb mol NaOH}}{40.0 \text{ lb NaOH}} \right| \frac{454 \text{ g mol}}{1 \text{ lb mol}} = 22.7 \text{ g mol}$
(b₂) $\frac{2.00 \text{ lb NaOH}}{1 \text{ lb}} \left| \frac{454 \text{ g}}{1 \text{ lb}} \right| \frac{1 \text{ g mol NaOH}}{40.0 \text{ g NaOH}} = 22.7 \text{ g mol}$

Check your answer. Convert the 2.00 Ib of NaOH to the SI system first, and then make the calculation.

EXAMPLE 2.2 Calculation of Molecular Weight

Since the discovery of superconductivity almost 100 years ago, scientists and engineers have speculated about how it can be used to improve the use of energy. Until recently most applications were not economically viable because the niobium alloys used had to be cooled below 23K by liquid He. However, in 1987 superconductivity in Y- Ba – Cu - O material was achieved at 90 K, a situation that permits the use of less expensive liquid N₂ cooling. What is the molecular weight of the following cell of a superconductor material? (The figure represents one cell of a larger structure.)



<u>Solution</u>

You can count the number of atoms of each element by examining Figure E2.1. Look up the atomic weights of the elements from the table in Appendix B. Assume that one cell is a molecule. By counting the atoms and carrying out the brief calculations below, you obtain the molecular weight of the cell.

Element	Number of atoms	Atomic weights	Mass (g)
Ba	2	137.34	2(137.34)
Cu	16	63.546	16(63.546)
0	24	16.00	24(16.00)
Y	1	88.905	1(88,905)
		Total	1764.3

The molecular weight of the cell is 1764.3 atomic masses/l molecule, or 1764.3 g/g mol. Finally, check your calculations.

Example:-2-3 Use of Molecular Weights to Convert Moles to Mass

How many pounds of NaOH are in 7.50 g·mol of NaOH?

Solution

The problem concerns converting g mol to lb. From Example 2.2, the MW of NaOH is 40.0.

Basis: 7.50 g mol of NaOH

 $\frac{7.50 \text{ g mol NaOH}}{454 \text{ g mol}} \frac{1 \text{ lb mol}}{454 \text{ g mol}} \frac{40.0 \text{ lb NaOH}}{1 \text{ lb mol NaOH}} = 0.661 \text{ lb NaOH}$

Note the conversion between Ib mol and g mol converts the value of 7.50 g mol the SI to the system of units. Could you first convert 7.50 g NaOH to g of NaOH, and then use the conversion of 454 g = 1 Ib to get lb NaOH? Of course.

2-4Flow rate:-

For continuous processes the flow rate of a process stream is rate at which material is transported through a pipe. In this book we usually use an overlay dot to denote a rate except for the volumetric flow rate F. **The mass flow rate** (\dot{m}) of a process stream is the mass (m) transported through a line unit time (t).

$$\dot{m} = \frac{m}{t}$$

The volumetric flow rate (*F*) of a process stream is the volume (*V*) transported through a line per unit time.

$$F = \frac{V}{t}$$

The molar flow (n) rate of a process stream is the number of moles (n) of a substance transported through a line unit time.

$$\dot{n} = \frac{n}{t}$$

Use any consistent units in your calculation.

<u>EXAMPLE 2.5</u> Application of Specific Gravity to Calculate Mass and Moles

In the production a drug having a molecular weight of 192, the exit stream from the reactor flows at a rate of 10.5 L/min. The drug concentration is 41.2% (in water), and the specific gravity of the solution is 1.024. Calculate the concentration of the drug (in kg/L) in the exit stream, and the flow rate of the drug in kg mol/min.

<u>Solution</u>: -

Read the problem carefully because this example is more complicated than the previous examples. You have a solution with some known properties including sp.gr. The strategy for the solution is to use the specific gravity to get the density from which you can calculate the moles per unit volume. After the problem, to make the requirements of the problem clearer, you should draw a picture, and put the given data on the picture. For the first part of the problem, you want to transform the mass fraction of 0,412 into mass per liter of the drug. Take 1.000 kg of the exit solution as a basis for convenience.



How do you get mass per volume (the density) from the given data, which is in terms of mass of drug per mass of solution (41.2%)? Use the specific gravity of the solution. Calculate the density as fonows

density of solution = $\frac{1.024 \frac{\text{g soln}}{\text{cm}^3}}{1.000 \frac{\text{g H}_2\text{O}}{\text{cm}^3}} \frac{1.000 \frac{\text{g H}_2\text{O}}{\text{cm}^3}}{\text{m}^3} = 1.024 \frac{\text{g soln}}{\text{cm}^3}$

Next convert the amount of drug in 1.000 kg of solution to mass of drug per volume of solution using the density

$$\frac{0.412 \text{ kg drug}}{1.000 \text{ kg soln}} \left| \frac{1.024 \text{ g soln}}{1 \text{ cm}^3} \right| \frac{1 \text{ kg}}{10^3 \text{ g}} \left| \frac{10^3 \text{ cm}^3}{1 \text{ L}} \right| = 0.422 \text{ kg drug/L soln}$$

Could you simplify the last two steps by knowing that 1.000 kg of water is 1.000 L? Certainly.

To get the flow rate, take a different basis, namely 1 minute.

Basis: 1 min = 10.5 L solution

Convert the volume to mass and then to moles using the information previously calculated.

 $\frac{10.5 \text{ L soln}}{1 \text{ min}} \frac{0.422 \text{ kg drug}}{1 \text{ L soln}} \frac{1 \text{ kg mol drug}}{192 \text{ kg drug}} = 0.023 \text{ kg mol/min}$

How might you check your answers?

1.5 Mole Fraction and Mass (Weight) Fraction

Mole fraction is simply the number of moles of a particular compound in a mixture or solution divided by the total number of moles in the mixture or solution. This definition holds for gases, liquids, and solids. Similarly, the mass (weight) fraction is nothing more than the mass (weight) of compound divided by the total mass (weight) of all of the compounds in the mixture or solution. Although the mass fraction the correct word, by custom ordinary engineering usage employs the term weight fraction. Mathematically, these ideas can be expressed as

mole fraction of
$$A = \frac{\text{moles of } A}{\text{total moles}}$$

mass (weight) fraction of $A = \frac{\text{mass of } A}{\text{total mass}}$

Mole percent and mass (weight) percent are the respective fractions times 100.

Example 2.6:- Conversion between Mass (Weight) Fraction and Mole Fraction

An industrial-strength drain cleaner contains 5.00 kg of water and 5.00 kg of NaOH. What are the mass (weight) fractions and mole fractions each component in the drain cleaner container?

Solution:-

You are given the masses so that it is easy to calculate the mass fractions. From these values you can then calculate the desired mole fractions.

A convenient way to carry out calculations in such conversion problems is to form a table, as shown below. Become skilled at doing so this type of problem and its inverse, that is, the conversion of mole fraction to mass fraction, will occur quite frequently. List the components, their masses, and their molecular weights in columns.

Component	kg	Weight fraction	Mol. Wt.	kg mol	Mole fraction
H ₂ O	5.00	$\frac{5.00}{10.0} = 0.500$	18.0	0.278	$\frac{0.278}{0.403} = 0.69$
NaOH	5.00	$\frac{5.00}{10.00} = 0.500$	40.0	0.125	$\frac{0.125}{0.403} = 0.31$
Total	10.00	1.000	3	0.403	1.00

Basis: 10.0 kg of total solution	Basis:
----------------------------------	--------

The kilogram moles are calculated as follows:

 $\frac{5.00 \text{ kg H}_2\text{O}}{18.0 \text{ kg H}_2\text{O}} = 0.278 \text{ kg mol H}_2\text{O}$

 $\frac{5.00 \text{ kg NaOH}}{40.0 \text{ kg NaOH}} = 0.125 \text{ kg mol NaOH}$

Adding these quantities together gives the total kilogram moles.

Example 2.7:- Nitrogen Requirements Used for the Growth of Cells,

In normal living cells, the nitrogen requirement for the cells is provided from protein metabolism (i.e., consumption the protein in the cells). When individual cells are commercially grown, $(NH_4)_2SO_4$ is usually used as the source of nitrogen. Determine amount of $(NH_4)_2SO_4$ consumed in a fermentation medium in which the final concentration is 35 g/L in a 500 L volume of the fermentation medium. Assume that the cells contain 9 wt. % N, and that $(NH_4)_2SO_4$ is the only nitrogen source.

Solution:-

Basis: 500 L solution containing 35 g/L

$$\frac{500 \text{ L}}{\text{ L}} \left| \frac{35 \text{ g cell}}{\text{ L}} \right| \frac{0.09 \text{ g N}}{1 \text{ g cell}} \left| \frac{1 \text{ g mol N}}{14 \text{ g N}} \right| \\ \times \frac{1 \text{ g mol } (\text{NH}_4)_2 \text{SO}_4}{1 \text{ g mol N}} \left| \frac{132 \text{ g } (\text{NH}_4)_2 \text{SO}_4}{1 \text{ g mol } (\text{NH}_4)_2 \text{SO}_4} \right| = 14,850 \text{ g } (\text{NH}_4)_2 \text{SO}_4$$

1- COMPOSITION:-

The composition of multicomponent solution and mixtures can be expressed as follow: -

a// weight fraction or weight percent:

weight (mass) fraction of $A = \frac{Mass \ of \ A}{total \ mass \ of \ mixture}$

Σ wt fraction = 1.000

weight % of A = wt fraction of $A \times 100$

$\Sigma wt \% = 100$

b// Mole fraction or mole percent

Mole fraction of $A = \frac{Moles \ of \ A}{total \ moles \ of \ mixture}$

 Σ mol fraction = 1.000

 $mol \% of A = mol \ fraction \ of \ A \times 100$

Σ mol % = 100

***Average molecular weight: -

The molecular weight of a mixture is known as average molecular weight (Mwt $_{mix}$) which can be estimated by two methods:

 $Mwt_{mix} = \frac{total \ mass \ of \ mixture}{total \ moles \ of \ mixture}$

 $Mwt_{mix} = Mwt_A y_A + Mwt_B y_B + Mwt_C y_C + \dots = \Sigma Mwt_i y_i$

Where: - y: mole fraction

c// Volume fraction or volume percent

Volume fraction of $A = \frac{Volume \text{ of } A}{total \text{ volume of mixture}}$

<u>Note:-</u>

Σ Vol fraction = 1.000 only for ideal solution

Σ Vol fraction \neq 1.000 for non – ideal solution

The following relation can be used to estimate the volume fraction of any component from its weight fraction which is useful with non-ideal solution

 $Volume \ fraction \ of \ A = \frac{Volume \ of \ A}{volume \ of \ mixture}$

$$Xv_A = \frac{V_A}{V_{mix}} = \frac{\frac{m_A}{\rho_A}}{\frac{m_{mix}}{\rho_{mix}}} = \frac{m_A \rho_{mix}}{m_{mix} \rho_A}$$

Sub. For the wt fraction of A (Xw_A) = $\frac{m_A}{m_m}$

$$Xv_A = \frac{Xw_A \quad \rho_{mix}}{\rho_A}$$

PA Where:- ρ_A : *density of A and* ρ_{mix} : *density of the mixture.*

<u>d// part per million (PPm) : -</u>

This term is used to express the weight or mole fraction of truce quantities of some components in the mixture. It is computed according to the relation:-

$$PPm of A = \frac{Mass or moles of A}{mass or moles of mixture} \times 10^{6}$$

It is commonly expressed in
$$mg/kg$$
 of mix or in $mol/10^6$ mol of mix

2- Concentration:-

Concentration is the term used to express the quantity of some solute in a unit volume of solution or in fixed amount of solvent it is expressed by the following terms:-

a// Mass Concentration:

It is the concentration expressed as the mass of solute per unit volume of the solution (gm solute/ liter, Ib_m solute/ft³, kg solute/m³, Ib_m solute/bbl).

b// Molarity (M):

It is the number of gram mole (mol) of solute dissolved in 1 liter of solution.

$$Molarity(M) = \frac{moles \ of \ solute}{Vol. \ of \ solution \ in \ liter}$$

Hence,

mole of solute = Molarity × Vol. of solution in liter

C// MolaLity:

It is the number of gram mole (mol) of solute dissolved in 1000 gm (1 kg) of solvent.

 $Molality = \frac{moles \ of \ solute}{mass \ of \ solvent \ in \ kg}$

d// Normality (N):

It is the number of gram equivalents of solute dissolved in 1 liter of solution.

Nolarity (N) =
$$\frac{gm \ equivalent \ of \ solute}{Vol. \ of \ solution \ in \ liter}$$

$$gm \ equivalent \ of \ solute = \frac{mass \ of \ solute \ in \ gm}{equivalent \ weight} = \frac{mass \ in \ gm}{\frac{M_{wt}}{Valancv}}$$

Nolarity (N) =
$$\frac{moles \ of \ solute}{Vol. of \ solution \ in \ liter} \times Valancy$$

Nolarity $(N) = M \times Valancy$

e// Parts per million by volume (PPm):

It is commonly used in very dilute aqueous solution (it is density nearly equals 1.0 gm/cm^3 or 1000 kg/m^3). Theme PPmv represent mg solute/liter of solution or gm solute/ m³ of solution.

Example 2.8:- Use of ppm

The current OSHA 8-hour limit for HCN in air is 10.0 ppm. A lethal dose of HCN in air is (from the Merck Index) 300 mg/kg of air at room temperature. How many mg HCN/kg air is 10.0 ppm? What fraction of the lethal dose is 10.0 ppm?

Solution:-

In this problem you have to convert ppm in a gas (a mole ratio, remember!) to a mass ratio.



Draw a simple picture. Put the data in the figure.



You can treat the 10.0 ppm as 10.0 g mol HCN/ 10^6 g mol air because the amount of HCN is so small when added to the air in the denominator of the ratio.

The 10.0 ppm is
$$\frac{10.0 \text{ g mol HCN}}{10^6 (\text{air} + \text{HCN}) \text{g mol}} = \frac{10.0 \text{ g mol HCN}}{10^6 \text{ g mol air}}$$

Next get the MW of HCN so that it can be used to convert moles of HCN to mass of HCN; the MW = 27.03.

Then

a.
$$\frac{10.0 \text{ g mol HCN}}{10^6 \text{ g mol air}} \left| \frac{27.03 \text{ g HCN}}{1 \text{ g mol air}} \right| \frac{1 \text{ g mol air}}{29 \text{ g air}} \left| \frac{1000 \text{ mg HCN}}{1 \text{ g HCN}} \right|$$
$$\times \frac{1000 \text{ g air}}{1 \text{ kg air}} = 9.32 \text{ mg HCN/kg air}$$
b.
$$\frac{9.32}{300} = 0.031$$

Does the answer seem reasonable? At least it is not more than 1!

Example 2.9:- Calculation of Mole Fraction and ppm from a Concentration in g/L

A solution of HNO₃ in water has a specific gravity of 1.10 at 25° C. The concentration of the HNO₃ is 15 g/L of solution. What is the

a. Mole fraction of HN0₃ in the solution?

b. ppm of HNO₃ in the solution?

Solution:-

Let the value of the specific gravity be the value of the density (ignoring any very minor effects related to the density of water).

	Basis:	1 L of solut	ior	n
15 g HNO ₃	1 L	1 cm ³		0 01264 g HNO3
1 L soln	1000 cm ³	1.10 g soln		g soln

Basis:	100	g so	lution
--------	-----	------	--------

The mass of water in the solution is: 100 - 0.0134 = 99.986 g H₂O.

the second se
< 10-5

Chapter 4: - Temperature

Temperature measuring scales used four types, two based on a relative scale degree Fahrenheit (°F) and Celsius (°C), and two based on an absolute scale degree Rankine (°R) and kelvin (K). Note that the degree symbol (°) not used with the kelvin temperature abbreviation K. Relative scales are the ones you hear the TV or radio announcer give. and are based on a specified reference temperature (32°F or 0 °C) that occurs in an ice-water mixture (the freezing point of water).

For recognize that the unit degree, the unit temperature difference or division) on the Kelvin-Celsius scale is not the same as that on the Rankine-Fahrenheit scale. If we $\Delta^{\circ}F$ represent the unit temperature difference in the Fahrenheit scale and $\Delta^{\circ}R$ be the unit temperature difference in the Rankine scale, and $\Delta^{\circ}C$ and ΔK be the analogous units in the other two scales, you probably are aware that

 $\Delta^{\circ} F = \Delta^{\circ} R$

 $\Delta^{\circ}C = \Delta K$

Also, if you keep in mind that the $\Delta^{\circ}C$ is larger than the $\Delta^{\circ}F$

$$\frac{\Delta^{\circ}C}{\Delta^{\circ}F} = 1.8 \quad \text{or} \quad \Delta^{\circ}C = 1.8 \; \Delta^{\circ}F$$
$$\frac{\Delta K}{\Delta^{\circ}R} = 1.8 \quad \text{or} \quad \Delta K = 1.8 \; \Delta^{\circ}R$$

Temperature measuring devices are of three types:

- 1- Thermal expansion (gas, liquid and bimetal thermometers)
- 2- Electrical measures: such as thermocouple which is based on the electromotive force (emf) developed between hot and cold junctions of two dissimilar metals. Thermistors are based on the change of electrical resistance with temperature.
- 3- Optical measures: such as pyrometer which is based on comparison of the color of object with that of a standard heated filament.

Thus, when we cite the temperature of a substance we are stating the cumulative number of units of the temperature scale that occur (an enumeration of ΔT_s)measured from the reference point. Reexamine Figure 4.1.







Figure 4.1 Temperatures scales.

$$T_{\rm *R} = T_{\rm *F} \left(\frac{1 \,\Delta^{\rm *}R}{1 \,\Delta^{\rm *}F} \right) + 460^{\rm *}R \tag{1.6}$$

$$T_{\rm K} = T_{\rm \circ C} \left(\frac{1 \,\Delta \rm K}{1 \,\Delta^{\circ} \rm C} \right) + 273 \,\rm K \tag{1.7}$$

$$T_{\rm ^oF} - 32^{\rm ^oF} = T_{\rm ^oC} \left(\frac{1.8 \ \Delta^{\rm ^oF}}{1 \ \Delta^{\rm ^oC}}\right) \tag{1.8}$$

$$T_{^{\circ}\mathrm{C}} = (T_{^{\circ}\mathrm{F}} - 32^{^{\circ}\mathrm{F}}) \left(\frac{1 \,\Delta^{^{\circ}\mathrm{C}}}{1.8 \,\Delta^{^{\circ}\mathrm{F}}}\right) \tag{1.9}$$
Principles ch.4

EXAMPLE 4.1 Temperature Conversion

Convert 100°C to (a) K, (b) °F, and (c) °R.

Solution

(a) $(100 + 273)^{\circ}C \frac{1 \Delta K}{1 \Delta^{\circ}C} = 373 \text{ K}$ or with suppression of the Δ symbol, $(100 + 273)^{\circ}C \frac{1 \text{ K}}{1^{\circ}C} = 373 \text{ K}$

(b) $(100^{\circ}C)\frac{1.8 \Delta^{\circ}F}{1 \Delta^{\circ}C} + 32^{\circ}F = 212^{\circ}F$ (c) $(212 + 460)^{\circ}F\frac{1 \Delta^{\circ}R}{1 \Delta^{\circ}F} = 672^{\circ}R$ or

$$(373 \text{ K}) \frac{1.8 \Delta^{\circ} \text{R}}{1 \Delta \text{K}} = 672^{\circ} \text{R}$$

EXAMPLE 4.2 Temperature Conversion

The heat capacity of sulfuric acid has the units J/(g mol)(°C), and is given by the relation

heat capacity = $139.1 + 1.56 \times 10^{-1}T$

where T is expressed in °C. Modify the formula so that the resulting expression has the associated units of Btu/(lb mol) (°R) and T is in °R.

Solution

The symbol °C in the denominator of the heat capacity stands for the unit temperature difference, $\Delta^{\circ}C$, not the temperature, whereas the units of T in the equation are in °C. First you have to substitute the proper equation in the formula to convert T in °C to T in °R, and then by multiplication by conversion factors convert the units on the righthand side of the equation to Btu/(lb mol) (°R) as requested.

heat capacity =
$$\left\{ 139.1 + 1.56 \times 10^{-1} \left[(T_{*R} - 460 - 32) \frac{1}{1.8} \right] \right\}$$

 $\times \frac{1 \text{ J}}{(\text{g mol})(^{\circ}\text{C})} \left| \frac{1 \text{ Btu}}{1055 \text{ J}} \left| \frac{454 \text{ g mol}}{1 \text{ lb mol}} \right| \frac{1^{\circ}\text{C}}{1.8^{\circ}\text{R}} = 23.06 + 2.07 \times 10^{-2}\text{T}_{*R}$

Note the suppression of the Δ symbol in the conversion between $\Delta^{\circ}C$ and $\Delta^{\circ}R$.

Example16:-

Convert 150 °C to °F, °R and K.

Solution:-

$$T_{\circ F} = 1.8 T_{\circ C} + 32 = 1.8(150) + 32 = 302 \circ F$$

 $T_{\circ R} = T_{\circ F} + 460 = 302 + 460 = 762 \circ R$
 $T_{K} = T_{\circ C} + 273 = 150 + 273 = 423 K$

Example17:-

Convert the heat transfer coefficient (h) of 200 Btu/ hr ft²°F to w/m² k. <u>Solution:-</u>

Example18:-

Show that: $T_{^{\circ}\mathrm{F}} = 2 \left[T_{^{\circ}\mathrm{C}} + \frac{1}{10} (160 - T_{^{\circ}\mathrm{C}}) \right]$

Solution:-

Chapter 5: - Pressure: -

Pressure is defined as the ratio of force to the area on which the force acts. Accordingly,

The pressure units are Ibf/in² (psi), dyne/cm² or N/m² (pascal).

Pressure is defined as "the normal (perpendicular) force per unit area." Examine Figure 5.1. Pressure is exerted on the top of the cylinder of mercury by the atmosphere, and on the bottom of the cylinder itself by the mercury, including the effect of the atmosphere.

The pressure at the bottom of the static (nonmoving) column of mercury exerted on the sealing plate is

$$p = \frac{F}{A} = \rho g h + p_0 \tag{5.1}$$

where p =pressure at the bottom of the column of the fluid

- F =force
 - A = area

 $\rho = \text{density of fluid}$

g = acceleration of gravity

h = height of the fluid column

 $p_0 =$ pressure at the top of the column of fluid

In the SI system the force is expressed in newtons, and area in square meters; then the pressure is N/m^2 or pascal (Pa). The value of the Pa is so small that the kilopascal (kPa) is a more convenient unit of pressure.



Figure 5.1 Pressure is the normal force per unit area. Arrows show the force exerted

On the respective areas.

It is convenient to introduce (g_c) in order to obtain the pressure unit.

Hence,
$$P_T = \frac{\rho g h}{g_c} + P_{\circ}$$

Some common nonstandard variations of pressure measurement used with the SI system are: -

- a. Bars (bar): 100 kPa = 1 bar
- b. Kilograms (force) per square centimeter (kg_f/cm²)*--a very common measure of pressure but not standard in SI (often called just "kilos")
- c. Torr (Torr): 760 Torr = 1 atm

In the AE system can be expressed in a variety of ways, including

- a. Millimeters of mercury (mm Hg)
- b. Inches of mercury (in. Hg)
- c. Feet of water (ft H_2O)
- d. Inches of water (in. H_2O)
- e. Atmospheres (atm)
- f. Pounds (force) per square inch (often just "pounds") (psi).

The pressure at a given position measured relative to absolute zero pressure or absolute vacuum is called the absolute pressure. Most pressure-measuring devices are calibrated to read zero in the atmosphere as shown in Figure 1.6.

These pressure gages indicate the difference between the absolute pressure and the local atmospheric pressure.

Pressures below atmospheric pressure are called vacuum pressures and are measured by vacuum gages that indicate the difference between the atmospheric pressure and the absolute pressure.

Absolute, gage, and vacuum pressures are all positive quantities and are related to each other by

$$P_{gage} = P_{abs} - P_{atm}$$
(5.2)

$$\mathbf{P}_{\rm vac} = \mathbf{P}_{\rm atm} - \mathbf{P}_{\rm abs} \tag{5.3}$$



Figure 1.6 Absolute, gage, and vacuum pressures.

Two common pressure units are the bar and standard atmosphere:

1 bar = 10^5 Pa = 0.1 Mpa = 100 kPa

1 atm = 101,325 Pa = 101.325 kPa = 1.01325 bar = 14.696 psi

<u>Measurement of Pressure:-</u>

Pressure, like temperature, can be expressed using either an absolute or a relative scale. Whether relative or absolute pressure is measured in a pressure measuring device depends on the nature of the instrument used to make the measurements. For example,

1. Manometers:-

Manometers are often used to measure moderate pressure. More accurate measurement of pressures below about 3 atm are provided by manometers. A manometer is a U- shaped tube partially filled with a fluid of known density known as the manometer fluid.

In general manometers are three types:-

- **<u>1</u> Open-end manometer: -** This manometer is used to measure a relative the *gauge pressure and degree vacuum* as shown in (Figure 5.2a) open-end manometer. Since the reference for the open end is the pressure of the atmosphere at the open end of the manometer.
- <u>2-</u> Closed –end manometer: This manometer is used to measure the absolute pressure as shown in (Figure 5.2b) closed-end manometer. When closing off the open end of the manometer and creating a vacuum in that end results in a measurement against a complete vacuum, or against "no pressure"; P_o in Equation (5.1) is zero. Such a measurement is called absolute pressure.





(b) Manometer measuring an absolute pressure.

<u>Note:</u> Mercury (Hg) is commonly used as a manometer fluid due to its higher density. The following relation can be used to compute the pressure in mmHg if other fluid is used:

$$\rho_m * h_m = \rho_{Hg} * h_{Hg}$$

Where: - ρ_m and h_m are the density and height of the fluid manometer.

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In contrast the zero point for a relative or gauge pressure measurement usually corresponds to the pressure of the air that surrounds us at all times, and as you know, varies slightly.

You are probably familiar with the barometer illustrated in Figure 5.3. Does a barometer read absolute or relative (gauge) pressure?



Figure 5.3 A mercury barometer.

<u>3-</u>

This manometer is used to measure the pressure difference between two points in a process line as shown in the figure. The general differential manometer equation is: -

$$P_1 - P_2 = \frac{(\rho_m - \rho) g h}{g_c}$$

Where: - ρ_m : density of the manometer fluid.

 ρ : density of the flowing fluid.

Special case: if the flowing fluid is a gas at moderate pressure, hence $\rho_m - \rho \approx \rho$ and the equation reduced to:

$$P_1 - P_2 = \frac{\rho_m \ g \ h}{g_c}$$



Figure 5.10 Concentric orifice used to restrict flow and measure the fluid flow rate with the aid of a manometer.

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2. <u>Mechanical gauges</u>: The most common type of this class is **Bourdon** gauge which normally measures relative pressure, but not always are used to measure fluid from nearly perfect vacuum to about 7000 atm. Figure 5.4 shows the workings of a dial device that measures pressure called *a Bourdon gauge*. Does it measure absolute or relative pressure?



Figure 5.4 Bourdon gauge pressure-measuring devices: (a) "C" Bourdon and (b) Spiral Bourdon.

EXAMPLE 5.1: - Pressure Conversion

The structures and dislocations in ceramic material determine the strength of the material in nanotechnology. Nonomaterials are more flexible than ordinary composites because each of the nanocrystallites (particles) can move past each other so that stretching can occur. However, nanosized particles can also enhance hardness. Crystallites pack together along the boundaries of macrocrystallites, and prevent the structure from unzipping. For example, a hardness in excess of 60 gigapascals has been reported for nanocrystals of titanium nitride embedded in thin films of silicon nitride. Hardness is measured by the pressure required to just indent the surface of a material (diamonds exhibit a hardness of greater than 100 Gpa). What is the equivalent pressure to 60 Gpa in

- a) atmospheres
- b) Psia
- c) inches of Hg
- d) rnm of Hg

Solution

For the solution, use the standard atmosphere.

Basis: 60 GPa
(a)
$$\frac{60 \text{ GPa}}{1 \text{ GPa}} \left| \frac{10^6 \text{ kPa}}{1 \text{ GPa}} \right| \frac{1 \text{ atm}}{101.3 \text{ kPa}} = 0.59 \times 10^6 \text{ atm}$$

(b) $\frac{60 \text{ GPa}}{1 \text{ GPa}} \left| \frac{10^6 \text{ kPa}}{1 \text{ GPa}} \right| \frac{14.696 \text{ psia}}{101.3 \text{ kPa}} = 8.70 \times 10^6 \text{ psia}$
(c) $\frac{60 \text{ GPa}}{1 \text{ GPa}} \left| \frac{10^6 \text{ kPa}}{1 \text{ GPa}} \right| \frac{29.92 \text{ in. Hg}}{101.3 \text{ kPa}} = 1.77 \times 10^7 \text{ in. Hg}$
(d) $\frac{60 \text{ GPa}}{1 \text{ GPa}} \left| \frac{10^6 \text{ kPa}}{1 \text{ GPa}} \right| \frac{760 \text{ mm Hg}}{101.3 \text{ kPa}} = 4.50 \times 10^8 \text{ mm Hg}$

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EXAMPLE 5.2: - Pressure Conversion

The pressure gauge on a tank of CO2 used to fill soda-water bottles reads 51.0 psi. At the same time the barometer reads 28.0 in. Hg. What is the absolute pressure in the tank in psia? See Figure E5.2.



Solution: -

The first thing to do is to read the problem. You want to calculate a pressure using convenient conversion factors, namely the standard atmosphere. Then examine Figure E5.2. The system is the tank plus the line to the gauge. All of the necessary data are known except what means. Is the pressure gauge reading psig not psia? Yes. You can assume the gauge is a Bourdon gauge measuring relative pressure, Equation (5.2) states that the absolute pressure is the sum of the gauge pressure and the atmospheric (barometric) pressure expressed in the same units. Let us change the atmospheric pressure to psia.

Atmospheric pressure =
$$\frac{28.0 \text{ in. Hg}}{29.92 \text{ in Hg}} = 13.76 \text{ psia}$$

The absolute pressure in the tank is

51.0 psia + 13.76 psia = 64.8 psia

Lastly, you always need to check, your answers. Try using a different conversion factor. You might first convert the barometric pressure to atm., then the gauge reading to atm. add the pressure in atm. and finally convert the result to psia. A long way to solve the problem. of course, but try it.

EXAMPLE 5.3: - Vacuum Pressure Reading

Small animals such as mice can live (although not comfortably) at reduced air pressures down to 20 KPa absolute. In a test, a mercury manometer attached to a tank, as shown in Figure E5.3, reads 64.5 cm Hg and the barometer reads 100 KPa. Will the mice survive?



Solution: -

First read the problem. You are expected to realize from the figure that the tank is below atmospheric pressure because the left leg of the manometer is higher than the right leg, which is open to the atmosphere. Consequently, to get the absolute pressure you subtract the 64.5 cm Hg from the barometer reading.

We ignore any corrections to the mercury density for temperature, and also ignore the gas density above the manometer fluid because it is much lower than the density of mercury. Then, since the vacuum reading on the tank is 64.5 cm Hg below atmospheric, the absolute pressure in the tank is

$$\mathbf{P}_{\rm vac} = \mathbf{P}_{\rm atm} - \mathbf{P}_{\rm abs} \tag{5.3}$$

$$100 \ kPa - 64.5 \ cm \ Hg \ \frac{101.3 \ KPa}{76.0 \ cm \ Hg} = 100 - 86 = 14 \ Kpa \ absolut$$

The mice probably will not survive.

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EXAMPLE 5.4: - Calculation of Pressure Differences

In measuring the flow of fluid in a pipeline as shown in Figure E5.4. a differential manometer was used to determine the pressure difference across the orifice plate. The flow rate was to be calibrated with the observed pressure drop (difference). Calculate the Pressure drop P1-P2 in Pascal for the manometer reading in Figure E5.4.



Solution: -

In this problem you cannot ignore the water density above the manometer fluid. Thus, we apply Equation (5.3) or (5.4), because the densities of the fluids above the manometer fluid are the same in both legs of the manometer. The basis for solving the problem is the information given in Figure E5.4. Apply Equation (5.4)

$$p_1 - p_2 = (\rho_f - \rho)gd$$

$$= \frac{(1.10 - 1.00)10^3 \text{ kg}}{\text{m}^3} \left| \frac{9.807 \text{ m}}{\text{s}^2} \right| \frac{(22)(10^{-3})\text{m}}{(\text{kg})(\text{m})} \left| \frac{1(\text{Pa})(\text{m}^2)}{1(\text{N})} \right|$$

$$= 21.6 \text{ Pa}$$

Check your answer. How much error would occur if you ignored the density of the flowing fluid?

EXAMPLE 5.5: - Pressure Conversion

Air is flowing through a duct under a draft of 4.0 cm H20. The barometer indicates that the atmospheric pressure is 730 mm Hg. What is the absolute pressure of the air in inches of mercury? See Figure E5.5



Solution: -

Can you ignore the density above manometer fluid and the air above the open end of the manometer? Probably. In calculations you must employ consistent units, and it appears in this case that the most convenient units are those of inches of mercury, so let's convert barometer reading and the manometer reading to in. using the standard atmosphere as the conversion factor.

Atmospheric pressure =
$$\frac{730 \text{ mm Hg}}{760 \text{ mm Hg}} = 28.7 \text{ in. Hg}$$

Next, convert 4.0 cm H₂O to in. Hg:

$$\frac{4.0 \text{ cm H}_2\text{O}}{2.54 \text{ cm}} \frac{1 \text{ fr}}{12 \text{ in.}} \frac{29.92 \text{ in. Hg}}{33.91 \text{ ft H}_2\text{O}} = 0.12 \text{ in. Hg}$$

Since the reading 4.0 cm H_{20} draft (under atmospheric), the absolute reading in uniform units is

$$P_{\text{vac}} = P_{\text{atm}} - P_{\text{abs}} \tag{5.3}$$

 $P_{abs} = P_{atm} - P_{Vac}$

(28.7 in. Hg) - (0.12 in. Hg) = 28.6 in. Hg absolute

Basis of calculation

Basis of calculation:-

It is necessary to choose and state a basis of calculations as the initial step of solution of any problem.

The proper choice of basis frequently makes the problem much easier to solve.

The basis is a specific quantity such as a certain period of time or a given mass of material which is selected as a reference for the calculations.

The following principle must be considered for suitable choice of the basis.

1- The basis must be fitted the available data, e.g. if the weight fractions are known, choose the total mass as a basis, and if the mole fractions are given, it is convenient to select the total number of moles as a basis.

يجب ان يكون الاساس يتناسب مع البيانات المتاحة

2- The quantity of material that is chosen as the basis must be neither small nor large numbers. The suitable basis is commonly 1 or 100 since the mass or number of moles of each component can be directly known from either the data of weight and mole fractions or wt. % and mol. % of the constituents.

كمية المادة التي يتم اختيار ها كأساس، يجب أن لا تكون أعداد(ارقام) صغيرة ولا كبيرة

3- A suitable unite time, i.e. hour, day, minuteetc., is frequently selected as the basis for continuous process.

في العمليةالمستمرة يتم تحديد الوقت كاساس مناسب مثل الساغة واليوم والدقيقة....الخ

- 4- If a quantity or flow rate of a certain stream in the process is given in the problem statement, it is usually most convenient to use this quantity as basis of calculation.
 إذا تم ذكر الكمية أو معدل تدفق تيار معين في العملية فالأنسب استخدام هذه الكمية كأساس للحساب.
- 5- If no stream amount or flow rates are known, it is better to choose the stream that contains most of substances involved in the processor the stream about which most informations are given (i.e. flow rate, composition etc.), as the basis of calculation.

التيار الذي يتم إعطاء معظم المعلومات حوله (مثل معدل التدفق أو التركيب ... إلخ) ياخذ كأساس في الحسابات.
 6- Sometime, it is convenient to solve the problem with basis an stream other than that of known flow rate in the problem due to the lacking of its data such as composition. The results of calculation is proportionally convert at the end of solution to the quantity given in the problem.

في بعض الاوقات، من المريح حل المشكلة <mark>مع أساس تيار آخر</mark> غير معدل التدفق المعروف في المشكلة <mark>بسبب نقص</mark> ب**ياناتها** مثل التركيب. ثم يتم تحويل نتائج الحسابات بالتناسب في نهاية الحل إلى الكمية المعطاة في المشكلة.

This common phenomena is known as "change of basis" which means shafting the basis in problem from one value to another for convenience in the calculations.

Example 3.1:-**Choosing a Basis**

The dehydration of the lower alkanes can be carried out using a ceric oxide (Ce O) catalyst. What is the mass fraction and mole fraction of Ce and O in the catalyst? Solution:

Start the solution by selecting a basis. Because no specific amount of material is specified, the question what do I have to start with does not help decide on a basis.

Neither does the question about the desired answer. Thus. Selecting a convenient basis becomes the best choice for a basis. What do you know about know Ce O? You from the formula that one mole of Ce is combined with one mole of O. Consequently, a basis of 2 kg mol. (or 2 g mol. or 2 lb mol. etc.) would make sense. You can get the atomic weights for Ce and O from Appendix B, and then you are prepared to calculate the respective masses of Ce and O in Ce O. The calculations are presented in the form of the following table:

Component	kg mol	Mole fraction	Mol. wt.	kg.	Mass fraction
Ce	1	0.50	140.12	140.12	0.90
0	1	0.50	16.0	16.0	0.10
Total	2	1.00	156.1	156.1	1.00

Basis: 2 kg mol of CeO

Choosing a Basis Example 3.2:-

Most processes for producing high- energy- content gas or gasoline from coal include some type of gasification step to make hydrogen or synthesis gas, Pressure gasification is preferred because of its greater yield of methane and higher rate of gasification. Given that a 50.0 kg test run of gas averages 10.0% H₂, 40.0% CH₄, 30.0% CO, and 20.0 % CO₂, what is the average molecular weight of the gas?

Solution

Let's choose a basis. The answer to question 1 is to select a basis of 50.0 kg of gas ("what I have to start with"), but is this choice a good basis? A little reflection will show that such a basis is of no use. You cannot multiply the given mole percent of this gas (remember that the composition of gases is given in mole percent unless otherwise stated) times kg and expect the result to mean anything. Try it, being sure to include the respective units. Thus, the next step is to choose a "convenient basis:' which is 100 kg mol., of gas, and proceed as follows:

Basis: 100 kg mol or Ib mol of gas

Set up a table such as the following to make a compact presentation of the calculations. You do not have to-you can make individual computations for each component, but such a procedure is inefficient and more prone to errors.

Component	Percent = kg mol or lb mol	Mol wt.	Kg or ib
CO,	20.0	44.0	880
co	30.0	28.0	840
CH₄	40.0	16.04	642
H ₂	10.0	2.02	20
Total	100.0		2382

Average molecular weight = $\frac{2382 \text{ kg}}{100 \text{ kg mol}}$ = 23.8 kg/kg mol

Check the solution by noting that an average molecular weight of 23.8 is reasonable since the molecular weights of the components varies from 10 to 40.

Example 3.4:- Calculation of the Mass Fraction of Components In Nanoparticles

The microstructure of nanosized particles has proved to be important in nanotechnology in developing economic magnetic performance of nanocomposites. In a ternary alloy such as $Nd_{4.5} Fe_{77}B_{18.5}$ the average grain size is about 30 nm. By replacing 0.2 atoms of Fe with atoms of Cu, the grain size can be reduced (improved) to 17 nm.

- (a) What is the molecular formula of the alloy after adding the Cu to replace the Fe?
- (b) What is the mass fraction of each atomic species in the improved alloy?

Solution

Pick a convenient basis. Because the atoms in the chemical formula of the alloy total to 100, pick a basis of

Basis: 100 g mol (or atoms) of Nd_{4.5}Fe₇₇B_{18.5}

- (a) The final alloy is Nd_{4.5} F_{76.8} B_{18.5} Cu_{0.2}
- (b) Use a table to calculate the respective mass fractions.

Component	Original g mol	Final g mol	MW	g	Mass fraction
Nd	4.5	4.5	144.24	649.08	0.126
Fe	77	76.8	55.85	4289.28	0.833
В	18,5	18.5	10.81	199,99	0.039
Cu		0.2	63.55	12,71	0.002
Total	100.0	100.0		5151.06	1.000

Example 3.5:- Changing Bases

A medium-grade bituminous coal analyzes as follows:

The residuum is C and H, and the mole ratio in the residuum is H/C = 9. Calculate the weight (mass) fraction composition of the coal with the ash and the moisture omitted (ash- and moisture-free).

Component	Percent
S	2
Ν	1
0	6
Ash	11
Water	3
Residuum	77

Solution:

To calculate the mass fractions of the components of the coal on an ash and moisture free basis, i.e., omitting the ash and water in coal in the list of compounds, you first have to determine the respective amounts of C and H in the residuum. Then you remove the ash and water from the list of compounds, add up the remaining masses, and calculate the mass fractions of each of the components remaining.

Take as a basis 100 kg of coal because then percent = kilograms.

Basis: 100 kg of coal

The sum of the S + N + O + ash + water is

$$2 + 1 + 6 + 11 + 3 = 23$$
 kg

You need to determine the individual kg of C and of H in the 77 kg total residuum.

To determine the kilograms of C and H. you have to select a new basis. Is 77 kg or 100 leg satisfactory? No. Why? Because the H/C ratio is given in terms of Moles, not weight (mass). Pick instead a convenient basis involving moles.

Basis: 100 kg mol.

Component	Mole fraction	kg mol	Mol. wt.	kg	Mass fraction	
Н	$\frac{9}{1+9} = 0.90$	90	1.008	90.7	0.43	
с	$\frac{1}{1+9} = \frac{0.10}{1.00}$	10	12	120 210.7	0.57	

On the basis of 100 kg of C+H, we have the kg of H and C, but we need to change the values to mesh with the basis of 100 kg of coal.

Basis: 100 kg of coal

The next step is to calculate the kg of C and H in the 77 kg of the residuum.

You can use the mass fractions from the table above, or just use the kg values directly:

H: (77kg) (0.43) = 33.15 kg C: (77 kg) (0.57) = 43.85 kg Finally, you can prepare a table summarizing the results on the basis of 1.00 kg of the coal ash-free and water-free.

Component	kg	Wt. fraction
С	43.85	0.51
Н	33.15	0.39
S	2	0.02
N	I	0.01
0	_6	0.07
Total	86.0	1.00

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Example 30:-

A gases mixture consists of three gases: argon, B and C. The analysis of this mixture is given as follow: 40.0 mol. % argon, 18.75 wt. %B and 20.0 mol. % C.

The molecular weight of argon: 40 and the molecular weight of C:50.

Calculate:

- a) The molecular weight of B.
- b) The average molecular weight of the mixture.
- c) The composition of the mixture as wt. %.

Solution:

a// Basis: 100 mol of the mixture.

No of mol. of $\operatorname{argon} = 40$ g mol. mass of $\operatorname{argon} = 40$ x 40 = 1600 gm. No of mol. of C = 20 gm mol. mass of C = 20 x 50 = 1000 gm. No of mol. of B = 100 - (40 + 20) = 40 gm mol.

Let molecular weight of $B = M_B$ mass of $B = 40 M_B$ gm.

Total mass of the mix. = $1600 + 1000 + 40 M_B = 2600 + 40 M_B$

wt. fraction of $B = \frac{Mass B}{Mass mix.} = \frac{40 M_B}{2600 + 40M_B} = \frac{18.75}{100} = 0.1875$

$$40 \text{ M}_{\text{B}} = 0.1875 (2600 + 40 \text{M}_{\text{B}})$$

$$40 \text{ M}_{\text{B}} - 7.5 \text{M}_{\text{B}} = 487.5$$
 $\therefore M_B = \frac{487.5}{32.5} = 15 \text{ molecular wt. of B}$

B// mol fraction of B = $\frac{40}{100} = 0.40$

$$M_{mix.} = \Sigma M_i y_i = 40(0.4) + 15(0.4) + 50(0.2) = 16 + 6 + 10$$

= 32 molecular wt of the mix.

Or

$$M_{mix.} = \frac{Total Mass}{Total moles} = \frac{2600 + 40(15)}{100} = \frac{3200}{100} = 32$$

C//

wt. % *argon* =
$$\frac{1600}{3200} x \, 100 = 50 \,\%$$
, *wt*. % *C* = $\frac{1000}{3200} x \, 100 = 31.25 \,\%$

Checking

 $\Sigma wt.\% = 50 + 18.75 + 31.25 = 100\%$

Example 31:-

A compound with molecular weight 119 consists of 70.6 wt. % C, 4.2 wt. % H, 11.8 wt. % N and 13.4 wt. % O. What is the chemical formula of this compound?

Solution 1:-

Basis: 1 gm mol. of compound

Mass = No of mol. x M wt. = $1 \times 119 = 119$ gm (70.6)

mass of
$$C = 119\left(\frac{70.6}{100}\right) = 84 \ gm \rightarrow \therefore \ gm \ atom \ C = \frac{84}{12} = 7 \ gm \ atoms$$

mass of $H = 119\left(\frac{4.2}{100}\right) = 5 \ gm \rightarrow \therefore \ gm \ atom \ H = \frac{5}{1} = 5 \ gm \ atoms$
mass of $N = 119\left(\frac{11.8}{100}\right) = 14 \ gm \rightarrow \therefore \ gm \ atom \ N = \frac{14}{14} = 1 \ gm \ atoms$
mass of $0 = 119\left(\frac{13.4}{100}\right) = 16 \ gm \rightarrow \therefore \ gm \ atom \ 0 = \frac{16}{16} = 1 \ gm \ atoms$

Chemical formula of the compound is C_7H_5NO

Solution 2:-

Basis: 100 gm of compound

mass of $C = 70.6 \ gm \rightarrow \therefore \ gm \ atom \ C = \frac{70.6}{12} = 5.88 \ gm \ atoms$
mass of $H = 4.2 \ gm \rightarrow \therefore \ gm \ atom \ H = \frac{4.2}{1} = 4.2 \ gm \ atoms$
mass of $N = 11.8 \ gm \rightarrow \therefore \ gm \ atom \ N = \frac{11.8}{14} = 0.84 \ gm \ atoms$
mass of $0 = 13.4 \ gm \rightarrow \therefore \ gm \ atom \ 0 = \frac{13.4}{16} = 0.84 \ gm \ atoms$
No of mol. of compound $= \frac{mass}{M_{wt}} = \frac{100}{119} = 0.84$ gm mole

gm mol. of	gm atoms	gm atoms	gm atoms	gm atoms
compound	С	Н	Ν	0
0.84	5.88	4.2	0.84	0.84
1	Х	Y	Z	W
	$X = \frac{5.88 \times 1}{0.84} = 7$	$Y = \frac{4.2}{0.84} = 5$	$Z = \frac{0.84}{0.84} = 1$	$W = \frac{0.84}{0.84} = 1$
The compound is C ₇ H ₅ NO				

Change the Basis to 1 gm mol. of compound

 $[\]frac{1}{Chemical formula of the compound is C_7H_5 NO}$

Principle ch.6

Example 32:-

Calculate the volume in gallons of benzene (C_6H_6) and ethylene dichloride ($C_2H_4Cl_2$) required to prepare 100 Ib of an ideal mixture composed of 20 mol.% C_6H_6 and 80 mol.% $C_2H_4Cl_2$.

Given that:

Components	Spg	Mwt.
C ₆ H ₆	0.872	78
$C_2H_4Cl_2$	1.246	99

Solution:

Solution 1 Basis: 100 Ib of the mixture

 $M_{mix.} = \Sigma M_i y_i = 78(0.2) + 99(0.8) = 15.6 + 79.2 = 94.8 molcular wt of the mix.$

No of moles of the mix. =
$$\frac{Mass}{Mwt.} = \frac{100 \text{ Ib}}{94.8 \frac{Ib}{Ibmole}} = 1.055 \text{ Ib mole}$$

mole of C6H6 = 1.055(0.2) = 0.211 lb mole \rightarrow mass of C6H6 = 0.21(78) = 16.45 lb mole of C2H4Cl2 = 1.055(0.8) = 0.844 lb mole \rightarrow mass of C2H4Cl2 = 0.844(99) = 83.55 lb Total = 100 lb

$$\rho_{C6H6} = spg * \rho_{water} = 0.872 * 8.34 \frac{lb}{gal} = 7.27 \frac{lb}{gal}$$

$$\rho_{C2H4Cl2} = spg * \rho_{water} = 1.246 * 8.34 \frac{lb}{gal} = 10.39 \frac{lb}{gal}$$

$$\therefore V = \frac{M}{\rho_{C6H6}} = \frac{16.45 \ Ib}{7.27 \ \frac{Ib}{gal}} = 2.26 \ gal$$
$$\therefore V = \frac{M}{\rho_{C2H4C12}} = \frac{83.55 \ Ib}{10.39 \ \frac{Ib}{gal}} = 8.04 \ gal$$

 \therefore Total Vol. of mix. = 2.26 + 8.04 = 10.30 gal

Solution 2 Basis: 100 Ib mole of the mixture

mol of benzen = 20 Ib mole
$$\rightarrow$$
 mass of benzen = 20(78) = 1560 Ib

mol of C2H4Cl2 = 80 Ib mole \rightarrow mass of C2H4Cl2 = 80(99) = 7920 Ib

∴ Total mass of mix. = 1560 + 7920 = 9480 Ib

$$\therefore Vol_{.C6H6} = \frac{Mass}{\rho_{C6H6}} = \frac{1560 \ lb}{7.27 \ \frac{lb}{gal}} = 214.6 \ gal$$
$$\therefore Vol_{.C2H4Cl2} = \frac{Mass}{\rho_{C2H4Cl2}} = \frac{7920 \ lb}{10.39 \ \frac{lb}{gal}} = 762.3 \ gal$$

Change the basis to 100 Ib

Mass mix (Ib)	gal C6H6	gal C2H4Cl2
9480	214.6	762.3
100	X	Y
	214.6 × 100	100 × 762.3
	$X = \frac{9480}{9480} = 2.26 \text{ gal}$	$Y = \frac{1}{9480} = 8.04 \ gal$

Example 33:

A solid mixture composed of NaCl and NaOH contains 40 Wt. % Na.

Calculate: a// The composition of the mixture as Wt. % NaCl & Wt. % NaOH.

b// The Wt.% of other elements (Cl, O and H) in this mixture.

	$Mwt. Of NaCl = 58.5 \qquad Mwt. Of NaOH = 40$
Solu	tion: Basis: 100 gm of the mixture
A//	Let mass of NaCl = (x)gm \rightarrow : moles NaCl = $\frac{X}{58.5}$ = 0.0171X mole
mas	$s of NaOH = (100 - x)gm \rightarrow \therefore moles NaOH = \frac{100 - X}{40} = (2.5 - 0.025 X) mole$
	Each mole of NaCl contains = 1gm atome of Na
and	Each mole of NaOH contains = 1gm atome of Na
	gm atoms of $Na = 0.0171X + 2.5 - 0.025X = 2.5 - 0.0079X$
	mass of $Na = (2.5 - 0.0079 X) 23 = 57.5 - 0.1817X = 40 gm$
	$\therefore X = \frac{57.5 - 40}{0.1817} = \frac{17.5}{0.1817} = 96.3 \ gm \ mass \ of \ NaCl$
	$\therefore 100 - 96.3 = 3.7 \ gm \ mass \ of \ NaOH$
	The mixture consists of 96.3 Wt. % NaCl & 3.7 Wt. % NaOH.
B//	\therefore No of mol of NaCl = 0.0171 X = 0.0171(96.3) = 1.646 mol
	\therefore No of mol of NaOH = 2.5 - 0.025 X = 2.5 - 2.408 = 0.092 mol
	\therefore gm atoms $Cl = No of mole of NaCl = 1.646 gm atoms$
	$mass Cl = 1.646 \times 35.5 = 58.44 \ gm$
	Similarly, $gm atom 0 = gm atom H = gm mole NaOH = 0.092 gm atom$
	$mass \ O = 0.092 \ \times 16 = 1.47 \ gm$
	$mass H = 0.092 \times 1 = 0.09 \ gm$
C	<i>Thacking:</i> Total mass of mix. = $40 + 58.44 + 1.47 + 0.09 = 100 \ gm$

∴ Composition of the mix. 40 Wt. % Na, 58.44 Wt. % Cl, 1.47 Wt. % O and 0.09 Wt. % H

Stoichiometry

<u> Stoichiometry: -</u>

The word stoichiometry (stoi-kiom- e-tri) derives from two Greek words: *stoicheion* (meaning "element") and *metron* (meaning "measure). Stoichiometry provides a quantitative means of relating the amount of products produced by chemical reaction(s) to the amount of reactants which are of great important in material and energy balance calculations.

As you already know, the chemical reaction equation provides both **qualitative** and **quantitative** information about the chemical reactions. Specifically the chemical reaction equation provides you with information of two types:

1. Stoichiometry coefficients:

The number that precede the chemical substances involved in the chemical reaction equation are a known as "Stoichiometry coefficients"

These coefficients represent the quantity of any reactant that is theoretically required for complete conversion of other reactants. That is mean "The coefficients of a balanced equation tell you what the mole ratios are among the substances that react or are produced".

2- تخبرك معاملات المعادلة المتوازنة بنسب المولات من بين المواد التي تتَّفاعل أو تنتج.

2. <u>Stoichiometry ratios:-</u>

The ratio between any stoichiometry coefficients in balanced chemical equation is known as "Stoichiometry ratios".

For example, the reaction of nitrogen & hydrogen to produce ammonia:

 $N_2 + 3H_2 \rightarrow 2NH_3$ The Stoichiometry ratios of $N_2/_{H_2} = 1/_3$ $N_2/_{NH_3} = 1/_2$ $H_2/_{NH_3} = 3/_2$

*****MMMMM*****

The total quantities of each of the elements on the left hand side equal those on the Right hand side. For example,

 $CH_4 + O_2 \rightarrow CO_2 + H_2O$

is not a balanced

is not a balanced stoichiometric equation because there are four atoms of H on the reactant side (left hand side) of the equation, but only two on the product side (right hand side). In addition, the oxygen atoms do not balance.

******** The balanced equation is given by

 $CH_4 + 2 O_2 \rightarrow CO_2 + 2 H_2O$ it is balanced 1 - C, 2 - H and 3 - OThe coefficients in the balanced reaction equation have the units of moles of a species reacting or produced relative to the other species reacting for the particular reaction equation.

If you multiply each term in a chemical reaction equation by the same constant, say two, the absolute stoichiometric coefficient in each term doubles, but the coefficients still exist in the same relative proportions.

Example 9.1:- Balancing a Reaction Equation for a Biological Reaction

The primary energy source for cells is the aerobic catabolism (oxidation) of glucose $(C_6H_{12}O_6 \text{ a sugar})$. The overall oxidation of glucose produces CO_2 and H_2O by the following reaction

 $C_6H_{12}O_6 + a O_2 \rightarrow b CO_2 + c H_2O$

Determine the values of a, b, and c that balance this chemical reaction equation.

<u>Solution:-</u>

Basis: The given reaction

By inspection, the carbon balance gives b = 6, the hydrogen balance gives c = 6, and an oxygen balance

$$6 + 2a = 6 \times 2 + 6$$

Gives a = 6. Therefore, the balanced equation is

 $C6H1206 + 602 \rightarrow 6C02 + 6H20$

Let's now write a general chemical reaction equation as: $c C + d D \rightleftharpoons a A + b B$ (9.1)

Where a, b, C, and d: are the stoichiometric coefficients for species A, B, C, and D, respectively, Equation (9.1) can be written in a general form

$$\nabla_A \mathbf{A} + \nabla_B \mathbf{B} + \nabla_C \mathbf{C} + \nabla_D \mathbf{D} = \Sigma \nabla_i S_i = 0$$
(9.2)

Where, V_i the stoichiometric coefficient for species S_i . The products are defined to have positive values for coefficients and the reactants to have negative values for coefficients. The ratios are unique for given reaction. Specifically in Equation (9.1)

$$V_c = -c$$
 $V_A = a$
 $V_D = -d$ $V_B = b$

If a species is not in an equation, the value of its stoichiometric coefficient is deemed to be zero. As an example, in the reaction:

$$\boldsymbol{0}_2 + 2\boldsymbol{C}\boldsymbol{O} \rightarrow 2\boldsymbol{C}\boldsymbol{O}_2$$

$$V_{02} = -1$$
 $V_{c02} = 2$

$$V_{co} = -2 \qquad \qquad V_{N2} = \mathbf{0}$$

Example 9.2: Use of the Chemical Equation to Calculate the Mass of Reactants Given the Mass of Products

In the combustion of heptane, CO_2 is produced. Assume that you want to produce 500 kg of dry ice per hour, and that 50% of the CO_2 can be converted into dry ice, as shown in Figure E9.2. How many kilograms of heptane must be burned per hour?



Solution:-

From the problem statement you can conclude that you want to use the product mass of CO_2 to calculate a reactant mass, the C_7H_{16} . The procedure is first to convert kilograms of CO_2 to moles, apply the chemical equation to get moles of C_7H_{16} , and finally calculate the kilograms of C_7H_{16} .

We will use Figure E9.2 the analysis. Look in Appendix DI to get the molecular weights of CO_2 (44.0) and C_7H_{16} (100.1). The chemical equation is:

 $C_7H_{16} + 11O_2 \rightarrow 7CO_2 + 8H_2O$

The next step is to select a basis.

Basis: 500 kg of dry ice (equivalent to 1 hr)

The calculation of the amount of C_7H_{16} can be made in one sequence:

 $\frac{500 \text{ kg dry ice}}{1 \text{ kg CO}_2} \frac{1 \text{ kg mol CO}_2}{0.5 \text{ kg dry ice}} \frac{1 \text{ kg mol CO}_2}{44.0 \text{ kg CO}_2} \frac{1 \text{ kg mol C}_7 \text{H}_{16}}{7 \text{ kg mol CO}_2}$ $\frac{100.1 \text{ kg C}_7 \text{H}_{16}}{1 \text{ kg mol C}_7 \text{H}_{16}} = 325 \text{ kg C}_7 \text{H}_{16}$

Finally, you should check your answer by reversing the sequence of calculations.

Limiting and excess reactants

1- Limiting and excess reactants:-

In most industrial processes, the quantities of reactants input are not in exact stoichiometric proportions as fixed by the reaction equation. It is generally desirable that same of the reacting materials be present in excess quantity over the amounts theoretically required for combination with other reactants.

a- *<u>The limiting reactant</u>* "is the reactant that is present in the smallest stoichiometric amount. It is theoretically disappear first if the reaction goes to completion according to the chemical equation and it has the smallest maximum extent of reaction:

(
$$\zeta$$
: GREEK SMALL LETTER ZETA)
 $\xi^{max} = \frac{Net \text{ moles input}}{Stoichiometry \text{ coef ficients}}$

[سیتم استهلاکه بالکامل] (The <u>limiting reactant:</u> would be completely consumed)

b- <u>The excess reactant</u>:" is the reactant that is present in excess amount over the Stoichiometric requirement equivalent to that limiting reactant and it has ξ^{max} higher than that of the limiting reactant.

As an example, if 10 moles of N_2 & 36 moles of H_2 are fed to the reactor for ammonia production.

$$N_2 + 3H_2 \rightarrow 2 NH_3$$

 $\xi_{N2}^{max} = \frac{10}{1} = 10$

$$\xi_{H2}^{max} = \frac{36}{3} = 12$$
 It has N₂ is the limiting reactant.

In another example, if 1.0 mole (A), 3.6 moles (B) and 3.0 moles (C) are fed to the reactor in which the following reaction is carried out:

$$A + 3B + 2C \rightarrow D$$

$$\xi_A^{max} = \frac{1}{1} = 1$$
 $\xi_B^{max} = \frac{3.6}{3} = 1.2$ $\xi_C^{max} = \frac{3}{2} = 1.5$

:. (A) is The Limiting reactant, B&C are the excess reactants.

c- Percent Excess:-

It is the excess quantity of any excess reactant expressed as a percentage of the Stoichiometric amount theoretically required to react completely with limiting reactant according to the chemical equation, i.e.

> $\% \ excess = rac{excess \ quantity}{theoretical \ amount} imes 100$ required

 $\% \ excess = rac{input - theo. \ amount \ required}{theoretical \ amount} \times 100$ required

For the previous examples

$$\% \ excess \ B = \frac{3.6 - 3}{3} \times 100 = 20 \ \%$$

% excess
$$C = \frac{3-2}{2} \times 100 = 50$$
 %

EXAMPLE 9.5 Calculation of the Limiting and Excess Reactants Given the Mass of Reactants

If you feed 10 grams of N2 gas and 10 grams of H2 gas into a reactor:

- a. What is the maximum number of grams of NH3 that can be produced?
- b. What is the limiting reactant?
- c. What is the excess reactant?

Г

Solution:-

You are asked to calculate the limiting reactant, and use a chemical reaction equation to calculate the NH3 produced. At room temperature and pressure no reaction will occur, but you are asked to calculate what would result if the reaction were to occur (as it does under other conditions of temperature and pressure), Look at figure E9.5.



The next step is to determine the limiting reactant by calculating the maximum extent of reaction based on the complete reaction of N2 and and H2.

$$\xi^{\text{max}}$$
 (based on N₂) = $\frac{-0.357 \text{ g mol N}_2}{-1 \text{ g mol N}_2/\text{moles reacting}} = 0.357 \text{ moles reacting}$

$$\xi^{\text{max}}$$
 (based on H₂) = $\frac{-4.960 \text{ g mol H}_2}{-3 \text{ g mol H}_2/\text{moles reacting}} = 1.65 \text{ moles reacting}$

You can conclude that (b) N2 is the limiting reactant, and that (c) H2 is the excess reactant. The excess H2 is 4.960 - 3(0.357) = 3.89 g mol. To answer question (a), the maximum amount of NH3 that can be produced is based on assuming complete conversion of the limiting reactant

4960 - 3(0357)	<u>N2</u>	<u>H2</u>
% excess H2 = $\frac{11000 - 3(0.007)}{3(0.357)} \times 100 = 363.2\%$	1	3
	0.357	Х
$0.357 \text{ g mol N}_{2}$ g mol NH ₂ 17.02 g NH ₂		
$\frac{1}{1 \text{ g mol N}_{2}} \frac{1}{1 \text{ g mol N}_{3}} \frac{1}{1 \text{ g mol N}_{3}} = 12.2 \text{ g NH}_{3}$	<u>N2</u>	<u>NH3</u>
	1	2
	0.357	Х

Conversion and degree of completion

2- Conversion and degree of completion:

In spite of using excess amount of some reactants, many industrial reactions do not go to completion part of the limiting reacted the other part remains unchanged.

a- <u>Degree of completion:</u>

Is the percentage (or fraction) of the limiting reactant that is actually Reacted and converted into products.

 $Fractional \ degree \ of \ completion = \frac{quantity \ reacted \ of \ the \ limiting \ reactant}{quantity \ input \ of \ the \ limiting \ reactant}$

b- <u>Conversion:</u>

Is the percentage (or fraction) of a specified reactant (usually the excess Reactant) that is actually reacted and converted into products.

$$\% Conversion = \frac{quantity of the substance that reactants}{quantity of the substance input} \times 100$$

Note:-

The quantity actually reacted is completed from the amount of product that is produced from the reaction.

For previous example

As an example, if 10 moles of N_2 & 36 moles of H_2 are fed to the reactor for ammonia production.

N2

1

Х

<u>H2</u>

3

Х

NH3

2

18

NH3

2

18

If 18 moles of ammonia is produced hence

$$N_2 + 3H_2 \rightarrow 2NH_3$$

 N_2 reacted = 18 (1/2) = 9 moles

 H_2 reacted = 18 (3/2) = 27 moles

Fractional degree of completion =
$$\frac{9}{10} = 0.9$$

% Conversion = $\frac{27}{36} \times 100 = 75\%$

For previous example

In another example, if 1.0 mole (A), 3.6 moles (B) and 3.0 moles (C) are fed to the reactor in which the following reaction is carried out:

$$A + 3B + 2C \rightarrow \mathbf{D}$$

IF 0.9 mole of (D) is produced, hence



% Conversion (B) =
$$\frac{2.7}{3.6} \times 100 = 75$$
 %

AND

% *Conversion* (*C*) =
$$\frac{1.8}{3} \times 100 = 60$$
 %

Yield

3- <u>Yield:-</u>

The can be defined as the ratio between the quantity (mass or moles) of the desired product obtained to the quantity of the key reactant fed. However, the percentage yield is defined as:

% yield = $\frac{quantity (mass or moles of the desired product formed}{theoretical quantity of the desired product that would be obtained} \times 100$ if the desired reaction had gaen to completion and there were no side reactions

No universally agreed upon definitions exist for yield-in fact- quite the contrary. Here are three common ones:

- Yield (based on feed}-the amount (mass or moles) of desired product obtained divided by the amount of the key (frequently the limiting) reactant fed.
- Yield (based on reactant consumed)-the amount (mass or moles) of desired product obtained divided by amount of the key (frequently the limiting) reactant consumed.
- Yield (based on theoretical consumption of the limiting reactant)-the amount (mass or moles) of a product obtained divided by the theoretical (expected) amount of the product that would be obtained based on the limiting reactant in the chemical reaction equation(s) if it were completely consumed.

Note: It is important to note that incomplete reactions and side reactions reduce the yield.

For the previous examples,

If 18 moles of ammonia is produced hence

$$N_2 + 3H_2 \rightarrow 2 NH_3$$

yield =
$$\frac{18 \text{ mol NH3}}{10 \text{ moles N2}} = 1.8 \text{ mol NH3/mol N2}$$

yield = $\frac{18 \text{ mol NH3}}{36 \text{ moles H2}} = 0.5 \text{ mol NH3/mol H2}$

H,0

EXAMPLE 9.6:- Yields in the Reaction of Glucose to Produce Ethanol

Yeasts are living organisms that consume sugars and produce a variety of products. For example, yeasts are used to convert malt to beer and corn to ethanol.

The growth of S- cerevisiae (a specific type of yeast) on glucose (a sugar) under anaerobic conditions (in the absence of oxygen) proceeds by the following overall reaction to produce biomass, glycerol, and ethanol.

$$C_6H_{12}O_6(glucose) + 0.118 \text{ NH}_3 \rightarrow 0.59 \text{ CH}_{1.74}N_{0.2}O_{0.45} \text{ (biomass)} + 0.43 C_3H_8O_3(glycerol) + 1.54 CO_2 + 1.3 C_2H_5OH \text{ (ethanol)} + 0.03$$

Calculate theoretical yield of biomass in g of biomass per g of glucose. Also, calculate the yield of ethanol in g of ethanol per g of glucose.

Solution:-

Basis: 0.59 g mol of biomass

0.59 g mol biomass	23.74 g biomass	1 g mol glucose	- 0.0779 a biamacala aluanza
l g mol glucose	1 g mol biomass	180 g glucose	- 0.0778 g biomass/g glucose
1.3 g mol C ₂ H ₅ OH	$46 \text{ g C}_2\text{H}_5\text{OH}$	1 g mol glucose	$= 0.332 \circ C_{\rm e} U_{\rm e} O H/\sigma \sigma has a $
l g mol glucose	1 g mol C2H5OH	180 g glucose	$= 0.332 \text{ g} C_2 H_3 OH g glucose$

4- Selectivity:-

It is the ratio of the moles of desired product produced to the moles of undesired product of produced in a set of reactions.

Note:

The terms "yield" and "selectivity" are terms that measure the degree to which a desired reaction proceeds relative to competing alternative (undesirable) reactions.

Selectivity = $\frac{\text{moles of desired product}}{\text{moles of undesired product}}$

Selectivity is the ratio of the moles of a particular (usually the desired) product produced to the moles of another (usually undesired or by-product) product produced in a set of reactions. For example, methanol (CH30H) can be converted into ethylene (C2H4) or propylene (C3H6) by the reactions

$$2 \text{ CH}_3\text{OH} \rightarrow \text{C}_2\text{H}_4 + 2\text{H}_2\text{O}$$
$$3 \text{ CH}_3\text{OH} \rightarrow \text{C}_3\text{H}_6 + 3\text{H}_2\text{O}$$

Of course, for the process to be economical, the prices of the products have to be significantly greater than the reactants. Examine the data in Figure 9.1 for the, concentrations of the products of the reactions. What is the selectivity of C2H4 relative to the C3H6 at 80% conversion of the CH3OH? Proceed upward at 80% conversion to get for C2H4 = 19 mole % and for C3H6 = 8 mole %. Because the basis for both values is the same, you can compute the selectivity 19/8 = 2.4 mol C2H4 per mol C3H6.



Figure 9.1 Products from the conversion of ethanol.

Principle ch.7

EXAMPLE 9.7: Selectivity in the Production of Nanotubes

A carbon nanotube may consist of a single wall tube or a number of concentric tubes. A single wall tube may be produced as unaligned structures or bundles of ropes packed together in an orderly manner. The structure of the nanotubes influences its properties, such as conductance. Some kinds are conductors and some semiconductors.

In nanotechnology, numerous methods (arc-discharge, laser vaporization, chemical vapor deposition, and so on) exist to produce nanotubes.

For example, large amounts of single wall carbon nanotubes can be produced by the catalytic decomposition of ethane over Co and Fe catalysts supported on silica

$$C_2H_6 \rightarrow 2C + 3H_2$$
 (a)
 $\Im C_2H_4 + H_2$ (b)

If you collect (3 g mol of H_2 and 0.50 g mol of C_2H_4 , what is the selectivity of C relative to C_2H_4 ?

Solution:

Basis: 3 g mol H₂ by Reaction (a) 0.50 g mol C2H4 by Reaction (b)

The 0.5 g mol of C2H4 corresponds to 0.50 g mol of H2 produced in Reaction (b).

Then the H2 produced by Reaction (a) was 3 - 0.50 = 2.5 g mol. Consequently, the nanotubes (the C) produced by Reaction (a) was (2/3)(2.5) = 1.67 g mol C

<u>С H2</u> 2 3 X 2.5

The selectivity was

1.67/0.50 = 3.33 g mol *C/* g mol C2H4

Example 34:-

Antimony obtained by heating pulverized stibnite (Sb2S3) with scrap iron and drawing off me molten antimony from the bottom of the reaction vessel.

 $Sb_2S_3 + 3Fe \rightarrow 2Sb + 3FeS$

Suppose that 600 gm of stibnite and 250 gm iron turnings are heated together to give 200 gm of Sb metal Determine:

(a) The limiting reactant, and the percentage of excess reactant

(b) % Conversion and fractional degree of completion.

(c) The yield, and

(d) Mass and composition (Wt. %) of reaction product.

Solution:-

A// moles of
$$Sb_2S_3 = \frac{600}{339.7} = 1.77$$
 mole $- - -$ moles of $Fe = \frac{250}{55.85} = 4.48$ mole

$$\xi_{Sb_2S_3}^{max} = \frac{1.77}{1} = 1.77 \qquad \qquad \xi_{Fe}^{max} = \frac{4.48}{3} = 1.49$$

Hence: Fe is The Limiting reactant and Sb₂S₃ is the excess reactant.

Theoretical Sb₂S₃ required =
$$4.48 (1/3) = 1.49$$

Sb2S3 Fe
1 3
X 4.48

% excess
$$Sb2S3 = \frac{input - theo.}{theo.} \times 100 = \frac{1.77 - 1.49}{1.49} \times 100 = 18.8 \%$$

B//

Sb produced = $\frac{200}{121.8}$ = 1.64 mol Fe reacted = 1.64 $\left(\frac{3}{2}\right)$ = 2.46 mol Sb₂S₃ reacted = 1.46 $\left(\frac{1}{2}\right)$ = 0.82 mol $\frac{5b2S3}{X} = \frac{Sb}{1}$ $\frac{Sb2S3}{X} = \frac{Sb}{1}$ $\frac{Sb2S3}{X} = \frac{Sb}{1}$

degree of completion
$$= \frac{Fe \ rected}{Fe \ input} = \frac{2.46}{4.48} = 0.55$$

Principle ch.7

$$\% Conversion = \frac{Sb2S3 \ rected}{Sb2S3 \ input} \times 100 = \frac{0.82}{1.77} \times 100 = 46.3 \ \%$$
(DEPEND ON THE EXCESS)

C//

$$Yield = \frac{200 \ gm \ Sb}{600 \ gm \ Sb2S3} = 1 \ gm \ Sb/3gm \ Sb2S3 \quad or \ 0.33gm \ Sb/3gm \ Sb2S3$$

D// Reaction product

Reaction product			
Component	mole	Mass, gm	Wt. %
Sb	1.64	200	23.5
FeS	1.64 (3/2)= 2.46	216	25.4
Sb ₂ S ₃ unreacted	1.77 - 0.82 = 0.95	322	37.9
Fe unreacted	4.48 - 2.46 = 2.02	112	13.2
		Total out= 850	100
Check input = 600+250 = 850			
Example 35:-

M wt.

Bauxite are containing 55.64 wt. % Al_2O_3 (the remainder being impurities) are reacted with sulfuric acid solution containing 78.4 wt. % H_2SO_4 to produced aluminum sulfate according to the following reaction:-

$$\begin{array}{rrrr} Al_2O_3 + 3H_2SO_4 & \to & Al_2(SO_4) + 3H_2O \\ 102 & 98 & 342 & 18 \end{array}$$

1100 Ib of bauxite with 2500 Ib of acid solution are fed to the process. The yield of this process is $[1.71 \ Ib \ Al_2(SO_4)/1 \ Ib \ of \ bauxite]$.

Calculate:

A. The limiting reactant, the excess reactant and % excess.

B. % Conversion and % degree of completion.

C. The mass and composition of reaction product.

Solution:-

$$Al_2O_3$$
 input = $1100\left(\frac{55.64}{100}\right) = 612 \ Ib - - No \ of \ moles = \frac{612}{102} = 6 \ Ib \ moles$

impuretes input =
$$1100\left(\frac{44.36}{100}\right) = 488 \ Ib = output \ quantity \ of \ impuretes$$

$$H_2SO_4 \text{input} = 2500\left(\frac{78.4}{100}\right) = 1960 \ Ib - -No \ of \ moles = \frac{1960}{98} = 20 \ Ib \ mole$$

Water input = $2500\left(\frac{21.6}{100}\right) = 540 \ Ib$
 $\xi_{Al_2O_3}^{max} = \frac{6}{1} = 6$ $\xi_{H_2SO_4}^{max} = \frac{20}{3} = 6.67$

Hence: Al₂O₃ is The Limiting reactant and H₂SO₄ is the excess reactant.

$\% \ excess \ H2SO4 = \frac{input - theo.}{theo.} \times 100 = \frac{20 - 18}{18} \times 100 = \frac{2}{18} \times 100 = 11.1 \ \%$				
Al_2SO_4 produced = 1.71(1100) = 1881 <i>Ib</i> \rightarrow <i>No of moles</i> = $\frac{1881}{342}$ = 5.5 <i>Ib mol</i>				
Al_2O_3 reacted = 5.5 lb mole \rightarrow % degree of completion = $\frac{5.5}{6} \times 100 = 91.7$ %				
H_2SO_4 reacted = 3 × 5.5 lb mole \rightarrow % Conversion = $\frac{16.5}{20}$ × 100 = 82.5 %				
Reaction product				
Component	Ib mole	Mass, Ib	Wt. %	
$Al_2(SO_4)_3$	5.5	1881	52.25	
Al ₂ O ₃ unreacted	6 - 5.5= 0.5	51	1.42	
H ₂ SO ₄ unreacted	20 - 16.5 = 3.5	343	9.53	
Water = (input+ produced)	540+(3x 5.5x 18)	837	23.25	
impurities		488	13.55	
		Total out=3600 Ib	100	
Check input = $2500+1100 = 3600$				

<u>Example 36:-</u>

Ethylene (C_2H_4) can be produced by dehydrogenation of ethane (C_2H_6). Methane can be produced as a by-product according the following reaction:

 $C_2H_6 \rightarrow C_2H_4 + H_2 ----(1)$ $C_2H_6 + H_2 \rightarrow 2CH_4 ----(2)$

The composition (mol. %) of the gaseous reaction product are as follow:

35 % C_2H_6 , 30% C_2H_4 , 28 % H₂ and 7 % CH₄

Calculate:

- A. The yield of C_2H_4 .
- **B.** Selection of C_2H_4 relative to CH₄.
- *C*. Feed molal ratio of C_2H_6 to H₂.

Solution:-	<u>C2H6</u>	<u>C2H4</u>
Basis: 100 mole of the reaction product	1	1
A// C_2H_4 produced = 30 mole, CH_4 produced = 7 mole	X	30
C_2H_6 reacted in both reaction = $30 + 7(1/2) = 33.5$ mole	<u>C2H6</u>	CH4
C_2H_6 unreacted (output) = 35 mole	1	2
C_2H_6 input = 33.5 + 35 = 68.5 mole	X	7

$$Yield = \frac{30 \text{ mole } C2H4}{68.5 \text{ mole } C2H6} = 0.44 \text{ mole} C2H4/mole C2H6}$$

B//

Selectivity =
$$\frac{30 \text{ mole } C2H4}{7 \text{ mole } CH4}$$
 = 4.29 mole C2H4/ mole CH4

C//

H2 produced from 1st reaction = C2H4 produced = 30 mole

H2 reacted in 2nd reaction = $\frac{1}{2}$ CH4 produced = $\frac{1}{2}$ (7) = 3.5 mole

H2 input + H2 produced from 1^{st} reaction = H2 reacted in 2^{nd} reaction +H2 output

H2 input + 30 = 3.5 + 28 H2 input = 31.5 - 30 = 1.5 mole

C2H6 input = 68.5

 $Feed ratio = \frac{68.5 \text{ mole } C2H6}{1.5 \text{ mole } H2} = 45.7 \text{ mole} C2H6/mole H2}$ <u>Home work: check total mass input & total mass output</u>

Example 37:-

It is required to produce chloropropene (C3H5Cl) from the reaction of propene with chlorine. Di-chloropropene ($C_3H_6Cl_2$) is also produced as side product.

$$C_3H_6 + Cl_2 \rightarrow C_3H_5Cl + HCl - - - - - (1)$$

 $C_3H_6 + Cl_2 \rightarrow C_3H_6Cl_2 \qquad ----(2)$

The following reaction product are recovered at the end of reaction:

Component	Cl_2	C ₃ H ₆	C ₃ H ₅ Cl	$C_3H_6Cl_2$	HCl
Ib mole	141.0	651.0	4.6	24.5	4.6

Calculate:

- A. Ib moles of $Cl_2 \& C_3H_6$ input to the reactor.
- **B.** The limiting reactant, excess reactant and % excess.
- C. Selectivity and the yield of C_3H_5Cl .

Solution:-

Basis: 1 batch

A// Cl_2 reacted in 1 st reaction = 4.6 Ibmole Cl₂ reacted in 2 nd reaction = 24.5 Ibmole

 Cl_2 unreacted = 141.0 Ib. mole

The total $Cl_2 = 4.6 + 24.5 + 141.0 = 170.1$ Ib. mole (*limiting*)

Similarly, total C_3H_6 input = 4.6 +24.5 + 651.0 = 680.1 Ib. mole (*excess*)

B// according to the main reaction, Cl_2 is the limiting reactant and C_3H_6 is the excess reactant.

$$\% \ excess_{C3H6} = \frac{input - theo.}{theo.} \times 100 = \frac{680.1 - 170.1}{170.1} \times 100 = 300\%$$

C//

yield =
$$\frac{C3H5 \ Cl \ produced}{C3H6 \ input} = \frac{4.6 \ lb \ mole}{680.1 \ lb \ mole}$$

= 0.0068 \ lb mole \C3H5Cl/ \ lb \ mole \C3H6
= 6.8 \ lb mole \C3H5Cl/ \ 1000 \ lb \ mole \C3H6

D//

Selectivity =
$$\frac{C3H5 \ Cl \ produced}{C3H6 \ input}$$
 = $\frac{4.6 \ Ib \ mole}{24.5 \ Ib \ mole}$
= 0.188 Ibmole C3H5Cl/ 1 Ib mole C3H6

Principle ch.7

Note:-

degree of completion =
$$\frac{Cl_2 \ rected}{Cl_2 \ input} = \frac{29.1}{170.1} = 0.171 \ (17.1\%)$$

% Conversion of C3H6 = $\frac{C3H6 \ rected}{C3H6 \ input} \times 100 = \frac{29.1}{170.1} \times 100 = 4.28 \%$ (DEPEND ON THE EXCESS)

These terms are meaning less due to the presence of the side reaction. It is more useful to compute

% Conversion of C3H6 to C3H5Cl = $\frac{4.6}{680.1} \times 100 = 0.68$ %

Principle ch.7

Example 3.10 Excess Air

Fuels for motor vehicles other than gasoline are being eyed because they generate lower levels of pollutants than does gasoline. Compressed propane has been suggested as a source of economic power for vehicles. Suppose that in a test 20 kg of C3H8 is burned with 400 kg of air to produce 44 kg of CO2 and 12 kg of CO. What was the percent excess air?

Solution:

This is a problem involving the following reaction (is the reaction equation correctly balanced?)

$$C_3H_8 + 5 O_2 \rightarrow 3CO_2 + 4H_2O$$

Basis: 20 kg of C3H8

Since the percentage of excess air is based on the complete combustion of C3H8 to CO2 and H2O, the fact that combustion is not complete has on influence on the definition of "excess air ". The required O2 is

<u>C3H8</u>	02
1	5
0.453	Х

The entering O2 is

400 kg air 1 kg mol. air 21 kg mol. O2 = 2.90 kg mol. O2 = 2.90 kg mol. O2

<u>Air</u>	02
100	21
20	х

The percentage excess air is

 $\frac{excess \ O2}{required \ O2} \times 100 = \frac{entering \ O2 - required \ O2}{required \ O2} \times 100$

% excess air = $\frac{290 \text{ kg mol } 02 - 2.27 \text{ kg mol } 02}{2.27 \text{ kg mol } 02} \times 100 = 28 \%$