B.sc I

Matarial Balance and process calculation
P - II
Semester - I

Unit and Dimensions

A Unit is an arbitrarily selected standard of measure for physical quntity.

physical quantity that can measured ~~as~~ always expressed as a product of its numerical value and units

physical quantity devided in two graups

- fundametal / basic such as length, mass, time
- derived quantities such as area, velocity and acceleration

system units devided as

- **Base Unit** – These units for basic quantities such as length, mass, time etc.
- **Derived unit** :- These are Units obtained by multiplying and dividing base units eg, cm^2 m/s, etc.

multiple units :- these are Unit which are multiple or fractions of base Units eq. hour, minute second etc.

Unit systems

Various systems of Units and basic quntities associated with them as given belaw

Fundamental quantity	System of Units				Dimension
	SI	MKS	CGS	FPS	
Length	meter (M)	meter (M)	centimeter cm	feet ft	L
Mass	kilogram Kg	Kilogram Kg	g	paund lb	M
Time	S	S	S	S	Q
Temperature	kelvin K	celsium °C	celsium °C	fahrenheit °F	T

Derived Units

The derived units are obtained from the base or fundamental unit using certain laws or definations.

→ ex. ① Volume is a products of three lengths

there fore unit of length is m

$V = l \times l \times l = l^3$ = unit is m^3

② pressure is defined as Force per unit area

$P = F/A = \frac{\text{Force}}{\text{Area}} = \frac{N}{m^2}$

Unit of pressure $= N/m^2$

Derived Quantity	Units	System of Units	Dimensions
Volumetric flow rate	Cubic meters per hour (m^3/h) Cubic centimeters per second (cm^3/s)	SI MKS	$L^3\theta^{-1}$ $L^3\theta^{-1}$
Volume	Cubic meters (m^3) Litres (l)	SI MKS	L^3 L^3
Density	Kilograms per cubic meter (kg/m^3) Grams per cubic centimeter (g/cm^3) Grams per millilitre (g/ml)	SI MKS CGS	ML^{-3} ML^{-3} ML^{-3}
Force	Newtons (N) Dynes (Dyne) Kilogram force (kgf)	SI CGS MKS	$ML\theta^{-2}$ $ML\theta^{-2}$ F
Pressure	Newtons per square meter (Pascals) [N/m^2, (Pa)] Kilograms force per square centimeter (kgf/cm^2)	SI MKS	$ML^{-3}\theta^{-2}$ FL^{-2}
Work / Energy	Joules (J) Meters kilogram force (m.kgf) Ergs (erg)	SI MKS CGS	$ML^2\theta^{-2}$ MF $ML^2\theta^{-2}$
Heat / Enthalpy	Joules (J) Kilocalories (kcal) Calories (cal)	SI MKS CGS	$ML^2\theta^{-2}$ $ML^2\theta^{-2}$ $ML^2\theta^{-2}$
Mass flow rate	Kilograms per hour (kg/h)	SI	$M\theta^{-1}$
Heat capacity	Joules per kilogram per degree Kelvin [J/(kg·K)] Kilocalories per kilogram per degree Celsius [kcal/(kg·deg C)]	SI MKS	$L^2\theta^2T^{-1}$ $L^2\theta^2T^{-1}$
Molar heat capacity	Joules per kilogram mole per degree Kelvin [J/(kmol·K)] Kilocalories per kilogram mole per degree Celsius [kcal/(kmol·deg C)]	SI MKS	$ML^2\theta^{-2}n^{-1}T^{-1}$ $ML^2\theta^{-2}n^{-1}T^{-1}$

Force ·

Force is proportional to the product of mass and acceleration

$$f \propto m \cdot a$$

$$f = k \cdot ma$$

Unit is Newton

work ·— is defined as product of the force acting on a body and distance travelled by the body in the direction of the applied force

$$W = F \cdot \times L$$

$$= kgf \cdot metre$$

$$= m\text{-}kgf$$

Some prefixes for the S I Units

1) giga (G) - multiply by ~~10~~ 10^9
2) mega (M) - multiply by 10^6
3) kilo K) — multiply by 10^3
4) milli (m) - multiply by 10^{-3}
4) Micro (μ) - multiply by 10^{-6}
5) nano (n) - multiply by 10^{-9}
6) deci (d) - multiply by 10^{-1}
7) deka (da) — // — 10^1
8) hecto (h) — // — 10^2
9) centi (c) — // — 10^{-2}

Conversion of Unit.

It is often neccesary to convert a physical quantity from one system of Unit to another.

example

		multiply by
Area	ft^2 — m^2	0.0929
	cm^2 — m^2	10^{-4}
Volume		
	ft^3 — m^3	10^{-6}
Velocity	ft/s — m/s	0.3048
mass		
	lb — kg	0.4536

Conversion factors to SI units :

To convert from	To	Multiply by
1. Length, L :		
ft	m	0.3048
cm	m	0.01
in	mm	25.4
in	m	0.0254
2. Area, L^2 :		
ft^2	m^2	0.0929
cm^2	m^2	10^{-4}
3. Volume, L^3 :		
ft^3	m^3	0.02832
cm^3	m^3	10^{-6}
l	m^3	10^{-3}
4. Velocity, L/θ :		
ft/s	m/s	0.3048
ft/h	m/s	8.467×10^{-5}
5. Volumetric flow rate, L^3/θ		
ft^3/s	m^3/s	0.02832
ft^3/h	m^3/s	7.867×10^{-6}
l/h	m^3/s	2×10^{-7}
l/s	m^3/s	10^{-3}
6. Mass, M :		
lb	kg	0.4536
t	kg	1000
g	kg	10^{-3}
7. Density, M/L^3 :		
lb/ft^3	kg/m^3	16.019
g/cm^3	$kg/m^3 = g/l$	1000
8. Mass flow rate, M/θ :		
lb/s	kg/s	0.4536
lb/h	kg/s	1.26×10^{-4}
9. Force, F :		
lbf	N	4.448
kgf	N	9.807
dyn	N	10^{-5}
10. Pressure, F/L^2 :		
lbf/ft^2	$N/m^2 = Pa$	47.88
std. atm	$N/m^2 = Pa$	1.01325×10^5
std. atm	kPa	101.325
in Hg	$N/m^2 = Pa$	3.386
in H_2O	$N/m^2 = Pa$	249.1
dyn/cm^2	$N/m^2 = Pa$	10^{-1}
mmHg	$N/m^2 = Pa$	133.3
torr	$N/m^2 = Pa$	133.3
bar	$N/m^2 = Pa$	10^5
kgf/cm^2	$N/m^2 = Pa$	9.808×10^4

Cont

1. Energy, work, heat, FL :		
cal	N·m = J	4.187
Btu	N·m = J	1055
kcal	N·m = J	4187
erg	N·m = J	10^{-7}
kW·h	N·m = J	3.6×10^6
. Enthalpy, FL/M :		
Btu/lb	(N.m)/kg = J/kg	2326
cal/g	(N.m)/kg = J/kg	4187
kcal/kg	(N.m)/kg = J/kg	4187
. Molar enthalpy, FL/mole		
Btu/lbmol	(N.m)/mol = J/mol	2326
cal/mol	(N.m)/mol = J/mol	4187
Heat capacity, specific heat, FL/MT :		
Btu/(lb · °F)	N.m/(kg·K) = J/(kg·K)	4187
cal/(g · °C)	N.m/(kg·K) = J/(kg·K)	4187
Molar heat capacity, FL/mole T :		
Btu/(lbmol · °F)	N.m/(kmol·K) = J/(kmol·K)	4187
cal/(mol · °C)	N.m/(kmol·K) = J/(kmol·K)	4187
Energy flux, FL/L²θ :		
Btu/(ft² · h)	N.m/(m² · s) = W/m²	3.155
cal/(cm²·s)	N.m/(m² · s) = W/m²	4.187×10^4
Power, FL/θ		
(ft·lbf)/s	(N.m)/s = W	1.356
hp	(N.m)/s = W	745.7
Btu/h	(N.m)/s = W	0.2931
kcal/h	(N.m)/s = W	1.163
Viscosity, M/Lθ		
P [poise ≡ g/(cm.s)]	kg/(m.s) = (N.s)/m²	0.10
cP	kg/(m.s) = (N.s)/m² = Pa·s	0.001
lb/(ft.s)	kg/(m.s)	1.488

While writing the units of fundamental or derived quantities, please remember the ing :

Correct : 10 kgf.m — incorrect : 10 kgfm

... two unit symbols should be separated by dot or space

Correct : 10 kg — incorrect : 10 kgs ... no plural form of the unit symbol

Correct : 10 cm — incorrect : 10 cm.

... no period/full stop at the end of the unit symbol

Correct : 10000 W/(m².K) — incorrect : 10000 W/m²·K

Correct : 10 kW — incorrect : 10 k W

... no space between the prefix symbol and the unit symbol

P A force of 19·635 kgf is applied on a piston of diameter 5.cm. find the pressure exerted on the piston in kpa

$$p = F/A$$

$$A = \frac{\pi}{4} d^2$$

$$A = \frac{\pi}{4} (5)^2$$

$$A = \frac{22 \cdot 7 \times 25}{4}$$

$$= 19{\cdot}635 \text{ cm}^2$$

$$p = \frac{19 \cdot 635}{19 \cdot 635} = 1 \text{ kgf} \cdot \text{cm}^{2}$$

$$= 1 \times \frac{101{\cdot}325}{1{\cdot}033227} \left[\frac{\text{kpa}}{\text{kgf/m}^2}\right]$$

$$= 98{\cdot}066 \text{ kpa}$$

pressure - pressure is defined as force per Unit area $p = f/A = \frac{\text{force}}{\text{Area}} = N/m^2 \text{ (pa) - SI}$
$= \text{kgf/cm}^2 \text{ - MKS}$

Types of pressure

1) atmospheric pressure
2) gage pressure (g)
3) Absolute pressure
4) Vacuum pressure

atmospheric pressure - The atmospheric pressure is the pressure that an area experiences due to the force exerted by atmosphere

$$1 \text{ atm} = 101{\cdot}325 \text{ k pa}$$
$$= 101325 \text{ N/m}^2 \text{ or pa}$$

or 1.033 kgf/m² — mks

gage pressure → is the pressure relative to the atmospheric pressure. In other words, how much above or below is the pressure with respect to with respect to the atmospheric pressure.

absolute pressure :- is the sum of atmospheric pressure and the gauge pressure

- If the gage pressure has a positive value the absolute pressure will be greater than the atmospheric pressure.
- If the gage pressure has a -ve value the absolute pressure will be less than the atmospheric pressure.

- it is also called as actual pressure
- Absolute pressure = Atmospheric pressure - vacuum
- Absolute pressure = Atmospheric pressure + gauge pressure

Vacuum pressure -

The pressure below the atmospheric pressure are called vacuum pressure measured by vacuum gauge

it is usually expressed in mm Hg or (torr) p· In a multiple effect evaporator system, the second effect is maintained under Vacuum of 475 MmHg (torr). find the absolue pressure in Kpa

Absolue pressure = atmospheric pressure - Vaccum

= 760 MmHg − 475

= 285 torr (mmHg)

= 285 mm Hg

1 atm = 101.325 Kpa

$= \frac{285 \times 101.325}{760} = 38$ Kpa

OR

=

mmHg converted to Pa multiply by 133.3

there for

$= 285 \times 133.3 = 37990.5$ pa

$= \frac{37990}{100} = 37.99$

= 38 Kpa

③ The force of 19.635 kgf is applied to piston of diameter 5cm find the pressure exerted on the piston kpa

$$p = \frac{F}{A}$$

$$A = \frac{\pi}{4} \times d^2$$

$$A = \frac{\pi}{4} \times (5)^2$$

$$A = 19.635 \, cm^2$$

$$p = \frac{19.635}{19.635} = 1 \, kgf/cm^2$$

∴ kgf/cm² is converted in kpa then multiply by $\frac{9.808 \times 10^4}{1000}$

$$1 \times \frac{9.808 \times 10^4}{103} =$$

$$1 \times 9.808 \times 10 = 98.080 \text{ kpa}$$

④ Convert pressure of 2atm to mm Hg

1 atm = 760 mm Hg

2 × 760 = 1520 mm Hg.

5) Convert Volumetric flow rate to $2 m^3/s$ to l/s

Sol/n $1 m^3 = 1000 l$

$\therefore m^3/s$ convert to l/s multiplied by 10^3

$2 \times 1000 = 2000 \ l/s.$

6) Convert 2000W in Hp — Unit of power

Conversion factor for.

Hp — W $(N.m)/s$

$Hp \times 745.7 = W$

$\therefore Hp = \frac{2000}{745.7} = 2.68 \ Hp.$

7) Convert 1000 dyen to Newton - (Force)

Conversion factor

dyn —— N

$dyn \times 10^{-5} = N$

$1000 \times 10^{-5} = N$

$0.01 = N$

8) Convert 1400 mm Hg to atm - (Pressure)

Sol/n. $atm \times 760 \ \overset{MMHg}{\cancel{MMHg}} = 1400 \ MMHg.$

$atm = \frac{1400}{760} = 1.842 \ atm$

Date

4) Convert 127 lb/ft³ to g/cm³ — **Density**

lb/ft³ to kg/m³ mult. by = 16.019

127×16.019 — kg/m³

= 2043.43 kg/m³

= 2043.43 kg/m³

cm³ — m³

$cm^3 \times 10^{-6}$ — m³

and g — kg

$g \times 10^{-3}$ = kg

kg — gm

$$= \frac{2043.43 \times 10^{-6}}{1000} = 2.034 \text{ g/cm}^3$$

mean.

$\frac{kg}{m^3} \longrightarrow g/cm^3$ multiplyed by 10^{-3}

C - 2

Basic chemical Calculation

Gram atom

It is defined as the mass in gram of an element which is numerically equal to its atomic weight

Gram atoms of an element

$$= \frac{\text{Weight in gram of an element}}{\text{atomic weight}}$$

Gram atom of element A

$$= \frac{\text{Weight in gram of A}}{\text{atomic weight of A}}$$

Kilogram atom of element A

$$= \frac{\text{Weight in kilogram of A}}{\text{atomic weight of A}}$$

Gram mole : It is defined as the mass in gram of a substance that is equal to numerically to its molecular weight.

Gram mole of comp B

$$= \frac{\text{Weight in gram of B}}{\text{molecular weight of B}}$$

Similarly kilogram comp of B

$$= \frac{\text{Weight in kilogram of B}}{\text{molecular wt of B}}$$

P. Calculate the kilogram atom of carbon which weight 36 kg.

Basis kg of carbon 36

Atomic weight of carbon = 12

$$\text{Katom of carbon} = \frac{\text{Weight in kg of carbon}}{\text{Atomic weight of carbon}}$$

$$= \frac{36}{12} = 3$$

P. Calculate the kilogram of 'Na' which the amount is specified as 3 K atom

soln

3 Katom 'Na'

Atomic weight of Na = 23

$$\text{Katom of Na} = \frac{\text{kg of Na}}{\text{Atomic weight of Na}}$$

$$3 = \frac{\text{Kg of Na}}{23}$$

Kg of Na = $23 \times 3 = 69$ Ans

P. Find the molecular weight.

i) H_2SO_4 ii) Na_2CO_3 iii) $KMnO_4$

$H_2SO_4 = 2\times1 + 1\times32 + 4\times16 = 98$

$Na_2CO_3 = 2\times23 + 1\times12 + 3\times36 = 106$

$KMnO_4 = 1\times39 + 1\times55 + 4\times16 = 158$

P How many Kilogram of ethane are there in 210 kmol

Base. 210 kmole ethane

soln ·K mole of ethane $= \frac{\text{Weight of kg in ethane}}{\text{molecular wt of ethane}}$

$$210 = \frac{\text{Weight in kg of ethane}}{\text{mol. wt of ethane}}$$

mol. wt of ethane

$= C_2H_6 = 2 \times 12 + 6 \times 1 = 30$

$$210 = \frac{\text{Weight in kg of ethane}}{30}$$

$210 \times 30 =$ Weight in kg of ethane

$6300 =$ " "

P Convert 88 kg of carbon dioxide into its amount in ~~molar~~ molar Units

soln Basis 88 kg of CO_2

mol. wt of CO_2 $= 12 \times 16 \times 2 = 44$

$$K\text{ mole of } CO_2 = \frac{\text{kg of } CO_2}{\text{mol. wt of } CO_2}$$

$$= \frac{88}{44} = 2$$

$= 2$ k mole of CO_2

P. Find mole of oxygen present for 500 gm

Basis - 500 gm of oxygen

$$\text{moles of } O_2 = \frac{\text{weight of } O_2}{\text{mol. wt of } O_2}$$

$$= \frac{500}{32} = 16.625 \text{ mol.}$$

P Convert 499 gm of $CuSO_4 \cdot 5H_2O$ into moles

Soln mol. wt of $CuSO_4$

= Cu = 65.5, S = 32 O = 16

$CuSO_4 \cdot 5H_2O$

$$= 63.5 + 32 + 64 + 5(2+16)$$

$$= 249.5$$

$$\text{moles of } CuSO_4 \cdot 5H_2O = \frac{499}{249.5} = 2 \text{ mol.}$$

Normality.

Number of gram-equivalent of solute dissolved in 1 lit of solution

it is denoted by (N)

$$\text{Normality} = \frac{\text{gram equivalent of solute}}{\text{Volume of solution in lit}}$$

molarity.

Number of gram moles of solute dissolved in one litre of solution

it is denoted by M

$$M = \frac{\text{gm moles of solute}}{\text{Volume of solution in litre}}$$

molality.

it is defined as Number of gram moles of solute dissolved in one Kilogram of solvent

$$\text{molality} = \frac{\text{gm moles of solute}}{\text{mass of solvent in kg}}$$

Concentration = Normality × equivalent weight

equivalent weight :- It is define as the ratio of the atomic weight or molecular weight to its valence.

The valence of an element or a compound depend on Number of Hydroxyl ion (OH^-) donated or Hyderogen ions H^+ accepted for each atomic weight or molecular weight

$$\text{equivalent weight} = \frac{\text{molecular weight}}{\text{Valence}}$$

Q 98 gm of Sulphuric Acid (H_2SO_4) are dissolved in water to prepare 1 lit of solution find Normality and Molarity

Sol^n Amount H_2SO_4 dissolved = 98 gm

mol. wt of H_2SO_4 = 98 gm

equivalent weight of H_2SO_4 = $\frac{\text{Mol. wt}}{\text{valance}}$

$= \frac{98}{2} = 49$

gm. equivalent of H_2SO_4 = ~~Mole~~ $\frac{\text{weight of } H_2SO_4}{\text{equivalent weight}}$

$= \frac{98}{49} = 2$

gm of equivalent

Normality $= \frac{2}{1} = 2$

Molarity = $\frac{\text{gm moles of solute}}{\text{~~molecular weight~~ volume of solution in L}}$

gm moles solute = $\frac{\text{weight of substance}}{\text{molecular weigh}}$

$= \frac{98}{98} = 1$

$M = \frac{1}{1} = 1$

p② 20 gm of Caustic soda is dissolved in water to prepare 500 ml solution find normality and molarity

soln -

Amount of caustic soda = 20 gm

molecular weigth = 40

equivalent weing $= \frac{\text{mol. wt}}{\text{Valence}} = \frac{40}{1} = 40$

volume of soln in lit = 500 ml

$= \frac{500}{100} = 0.5$ lit.

Normality $= \frac{\text{gm-equivalent NaOH}}{\text{Volume of sol}^n \text{ in lit}}$

gm.eq. of NaOH $= \frac{20}{40} = 0.5$ gmeq.

$= \frac{0.5}{0.5} = \underline{\underline{1}}$

molarity $= \frac{\text{gram mole of NaOH}}{\text{Volume of sol}^n \text{ in lit}}$

gram moles of NaOH $= \frac{\text{weigth of substance}}{\text{molecular weight}}$

$= \frac{20}{40} = 0.5$

molarity $= \frac{0.5}{05} = \underline{\underline{1}}$

P. Find gram of HCl needed to prepare 1 lit 2N HCl solution.

Basis. 1 lit 2N HCl soln

$$\text{Normality} = \frac{\text{gram eq. of HCl}}{\text{Volume of solution lit}}$$

$$2 = \frac{\text{gm eq of HCl}}{1}$$

Equivalents of HCl = 2 gm-eq

$$\text{gm equivale} = \frac{\text{Weight of substance}}{\text{equivalent weight}}$$

$$2 = \frac{\text{Weight of substance}}{36.5}$$

$$36.5 \times 2 = \text{Weight of substance}$$

$$73 \text{ gm} = \text{〃}$$

P. The concentration of an aqueous solution of acetic acid is specified as 30% on weight basis. Find the molality of solution.

Basis
100 kg of solution

Amount of Acetic Acid in it = 30 kg

Amount of Water solvent = 70 kg.

Amount of acetic Acid in gm = 30×10^3 gm molecular weight of CH_3COOH = 60

gm. moles of Acetic Acid $= \dfrac{\text{Weight of acid}}{\text{Mol. wt}}$

$= \dfrac{30 \times 10^3}{60} = 500$ mole

Molality of solution $= \dfrac{\text{moles of acetic acid}}{\text{Kg of solvent}}$

$= \dfrac{500}{70} = 7.142$ ✓

P- A solution of caustic soda contain 20% NaOH taking density of the solution 1.196 Kg/l find normality, Molarity and molality of solution

Solution → Volume of soln – 100 Kg.

The solution contain 20% NaOH.

means

20 Kg of NaOH

and 80 Kg of Solvent

Density = 1.196 Kg/lit

Normality of NaOH $= \dfrac{\text{gm equivalent}}{\text{Volume of soln. in Lit}}$

gm. equivalent of NaOH $= \dfrac{\text{Weight of substance}}{\text{equivalent wt}}$

$= \dfrac{20\,\text{kg}}{40} = 0.5.$

$= \dfrac{20 \times 10^3}{40} = 500$.

∴ Volume of solution is 100 kg It's convert into litre

∴ density $= \frac{\text{mass}}{\text{volume}}$

Volume $= \frac{\text{mass}}{\text{density}} = \frac{100 \text{ kg}}{1.196 \text{ kg/lit}}$

$= \underline{\underline{83.61}}$ litre

Normality $= \frac{500}{83.61} = 5.98$

Normality = molarity = 5.98

∴ mol.wt = eq.wt of NaOH.

Molality $= \frac{\text{gram moles of NaOH}}{\text{kg of solvent}}$

$= \frac{500}{80} = 6.25$ mol/kg.

P. H_2SO_4 solution has a molarity 11.24 and molality of 94. Calculate the density of solution

<u>Sol</u>

Sol^n consider soln is 1 lit

given molarity = 11.24

Molality = 94

molarity $= \frac{\text{gm moles } H_2SO_4}{\text{Volume of soln in lit}} = 11.24 = \frac{gm.M}{1}$

$11.24 = \frac{\text{gm moles of } H_2SO_4}{1}$

$= 11.24$

~~Weight of substance =~~

gm mole of $H_2SO_4 = \frac{\text{weight of substance}}{\text{molecular weight}}$

$11.24 \times 98 =$ ~~weight of substance~~

1101.52 gm = weight of substance

~~1.101 kg = substance weight~~

Molality $= \frac{\text{gm-moles of substance}}{\text{Volume of solvent in kg}}$

$94 = \frac{11.24}{\text{Volume of solvent in kg}}$

Volume of solvent in kg = ~~94 × 11.24~~ $\frac{11.24}{94}$

$= 0.1195$ kg

~~Volume~~/ Amount of solution = 1.101 + 0.1195

= 1.2205 kg.

Density $= \frac{\text{Mass}~~\text{Volume}~~}{~~\text{Mass}~~\ \text{Volume}} = \frac{1.2205}{1}$

= 1.2205 kg/lit.

Method of expressing the composition of mixtures and solution.

The composition of mixture or solution can be expressed in weight percent, volume percent and mole percent.

The composition of solid and liquid in expressed in term of weight percent and mole percent.

The composition of gases is expressed in term of volume percent.

Weight percent :

It is the weight of any component expressed as percentage of total weight of the system.

$$\text{Weight \% of A} = \frac{\text{Weight of A}}{\text{total weight of system}} \times 100$$

$$= \frac{W_A}{W} \times 100$$

$W = W_A + W_B$ — weight of system

W_A = weight of component 'A

Volume percent

It is a pure component volume of any component expressed as a percentage of the total volume of the system

$$\text{Volume \% of A} = \frac{\text{pure component volume of A}}{\text{Total volume of system}} \times 100$$

$$= \frac{V_A}{V} \times 100$$

V_A = pure component volume of A

V = Total volume of system $V_A + V_B$

Mole percent :

It is mole of component expressed as a percentage of the total moles of the system

$$\text{mole \% of A} = \frac{\text{moles of A}}{\text{Total moles of system}} \times 100$$

$$= \frac{\frac{W_A}{M_A}}{\frac{W_A}{M_A} + \frac{W_B}{M_B}} \times 100$$

Where M_A and M_B are the molecular weights of component A & B respectively.

Mole fraction :

It is the ratio of the Number of moles of a particular component to the total moles of system for binary system A and B

$$\text{mole fraction of A} = \frac{\text{Moles of A}}{\text{Total moles of system}}$$

$$x_A = \frac{\frac{W_A}{M_A}}{\frac{W_A}{M_A} + \frac{W_B}{M_B}} \quad \text{— ①}$$

x_A = Mole fraction of A

x_B = mole fraction of B

$$X_B = \frac{\frac{W_B}{M_B}}{\frac{W_A}{M_A} + \frac{W_B}{M_B}} \quad —②$$

mole % of A = mole fraction A × 100

adding ① and ② we get

$$X_A + X_B = \frac{\frac{W_A}{M_A}}{\frac{W_A}{M_A} + \frac{W_B}{M_B}} + \frac{\frac{W_B}{M_B}}{\frac{W_A}{M_A} + \frac{W_B}{M_B}}$$

$$= \frac{\frac{W_A}{M_A} + \frac{W_B}{M_B}}{\frac{W_A + W_B}{M_A \quad M_B}} = 1$$

Sum of mole fraction all the component present in a given system is equal to Unity

$$\sum_{i=1}^{n} x_i = 1.0$$

Sum of all mole % for given system total a 100

Date / /

P. an aqueous soln of sodium chloride is prepared by dissolving 25 kg of sodium chloride in 100 kg water.

Determine (a) weight % and mole % composition of solution

Soln

Amount of solution

25 kg of NaCl + 100 kg water

= 125 kg

Weight % of NaCl $= \frac{\text{kg of NaCl}}{\text{kg of solution}} \times 100$

$= \frac{25}{125} \times 100 = 20$

Weight % H_2O $= \frac{100}{125} \times 100$

= 80 %

mol. wt of NaCl = 58.5

mol. wt of H_2O = 18

moles of NaCl $= \frac{25}{58.5} = 0.427$ K mol

moles of H_2O $= \frac{100}{18} = 5.56$ k mol.

Total moles of solution = 0.427 + 5.56

= 5.987 k mol.

mole % of NaCl solution

$$= \frac{\text{Kmol NaCl}}{\text{Kmol solution}} \times 100$$

$$= \frac{0.427}{5.987} \times 100$$

$$= 7.13$$

mole % H_2O in solution

$$= 100 - \text{mole \% NaCl}$$

$$= 100 - 7.13$$

$$= 92.87 \%$$

OR

$$= \frac{\text{K mole of } H_2O}{\text{K mole of solution}} \times 100$$

$$= \frac{5.56}{5.987} \times 100$$

$$= \underline{92.87}$$

P→ sodium chloride weighing 200 kg is mixed with 600 kg potassium chloride calculate the composition mix in (i) weight % and (ii) mole %.

<u>Soln</u>

weight of NaCl in mixture = 200 kg
weight of KCl in mixture = 600 kg
Total weight of mix = 800 kg

Ideal gas Law

There are several ways to derive the Ideal Gas Law but the simplest way to use the three Simple gas Law

Avogadro's Law

- State that Volume of a gas is directly proportional to the Number of moles.

$$V \propto n$$

Boyle's Law - State that the volume of a gas is inversely proportional to its pressure

$$V \propto \frac{1}{P}$$

Charles's Law

State that the volume of a gas is directly proportional to its Kelvin temperature

$$V \propto T$$

We combine these three equation we get

$$V \propto \frac{nT}{P}$$

$$\therefore V = K\frac{nT}{P}$$ K is proportionality constant

We replace K with Universal gas consta

We get $V = \frac{RnT}{P}$

: $PV = nRT$

P: absolute pressure kpa
V in m^3 and T - temp in kelvin.
and n - k mole

The Unit of $R = \frac{m^3 \cdot kpa}{kmol \cdot K}$

Value = 8.31451

Unit $R = \frac{kcal}{kmol \cdot K} = 1.987$

$R = \frac{J}{mol \cdot K} = 8.31451$

P. Calculate the volume occupied by 20kg of chlorine gas at a pressure of 100 k pa and 298 K (25°c)

Cal

basis 20kg of Cl_2 gas

$PV = nRT$

$$V = \frac{nRT}{P}$$

$$V = \frac{n \times 8.31451 \times 298}{100}$$

n = no. of moles = $\frac{\text{Weight of substance}}{~~100~~ \; 71 \, (M.W)}$

$= \frac{20}{71} = 0.2817$ kmol

$= \frac{0.2817 \times 8.31451 \times 298}{100} = 6.98 m^3$

P. 15 kg of carbondioxide is a compressed at a temp of 303 K (30°c) to a Volume of 0.5 m^3 Calculate the pressure required for given duty Assume ideal gas Law is applicable

Soln 15 kg of CO_2

$$PV = nRT$$

$$P = \frac{nRT}{V}$$

$$n = \text{no. of moles} = \frac{15}{44} = 0.341 \text{ Kmol}$$

$$P = \frac{0.341 \times 8.31451 \times 303}{0.5}$$

$$= \underline{1718.16 \text{ kpa}}$$

P. 5 kg of oxygen containing is a closed container of volume 1 m^3 is heated without exceeding a pressure of 709.28 Kpa. Calculate maximum Temp in gas attained

Basis · 5 kg of oxygen

mol.weight O_2 = 32

$$\text{moles of } O_2 = \frac{5}{32} = 0.1562 \text{ Kmol}$$

$$PV = nRT$$

$$T = \frac{PV}{nR}$$

$$= \frac{709.28 \times 1}{0.1562 \times 8.31451} = \underline{\underline{543.13K}}$$

$$= 543.13K - 273 = \left(\underline{273.13 °c}\right)$$

P Calculate the weight of 1 m^3 of chlorine gas at a temperature of 298 K (25°C) and pressure of 101·325 Kpa (1 atm)

Soln 1 m^3 Cl_2 gas

$$PV = nRT$$

$$\therefore n = \frac{PV}{RT}$$

$$= \frac{101.32p \times 1}{8.31451 \times 298}$$

$$= 0.0409 \text{ kmol}$$

no. moles = $\frac{\text{weight of sub.}}{\text{mol. wt}}$

Weight of substance = no. moles × mol wt

= 0.0409 × 71 = 2.904 kg

C - 3

Material balance without chemical Reaction

A chemical process is required to carry out of raw material into product effectively and economically. Material and energy balance calculation is required for desired product. It is help us (i) to evaluate specific consumption of material (ii) to evaluate losses of materials and energy (iii) to find out reasion for malfunctioning of processing unit.

Outline of a Procedure for Material Balance Calculations :

(1) Assume a suitable basis of calculation such as quantity or flow rate of the entering or leaving stream. If basis is not specified in the statement of the problem, assume a new convenient basis (quantity or flow rate of a suitable stream of which the composition data is given).

(2) Adopt weight units such as grams or kilograms in case of problems of processes without chemical reactions (i.e., wherein no chemical reactions occur) and adopt/use molar units such as gram moles or kilogram moles in case of problems of processes with chemical reactions, i.e., involving chemical reactions as far as possible for the purpose of simplification.

(3) Draw a block diagram of the process wherein each operation is represented by a rectangular block wherein the input and output streams are represented by an inflow and outflow arrow.

(4) In the block diagram drawn, indicate the information provided regarding the input and output streams given in the problem statement such as quantity, flow rate, composition, materials, etc.

(5) Search out the unknown quantities or composition, flow rates, etc.

(6) Search out the unknowns involved in the problem and ascertain them some x, y, z, etc. (depending upon a number of unknowns) and generate, with the help of data given, the material balance equations in terms of x, y, z, etc. equal to the number of unknowns. Equations can be generated (independent) by making the overall material balance and individual material balance of components involved and solve them.

(7) In case of problems involving a chemical reaction, write a balanced chemical equation, search out a limiting component and so on - as the quantities produced during the chemical reaction or components reacted/consumed are to be calculated on the basis of the limiting reactant reacted and the chemical reaction under consideration.

Ma

It means that

Input = out put

ex. A is a solid

A input to the reactor = A out put from the Reactor + A unreacted

or

Accumulation

Distillation:.

This operation Is used for the Separation of the components of a liquid mixture by partial Vaporization and condensation

Distillation with rectification or (Fractional Distillation) gives almost pure product. the product removed from the top is called as distillate or overhead product and that removed from bottoms or bottom product. Material is generally based on the more Volatile component.. the vapour phase is created by suplying thermal energy to the liquid to be distillate and this method of seperation depends on the difference in Vapour pressure of different component at a given temperature.

Block diagram of distillation operation for binary System of (A+B)

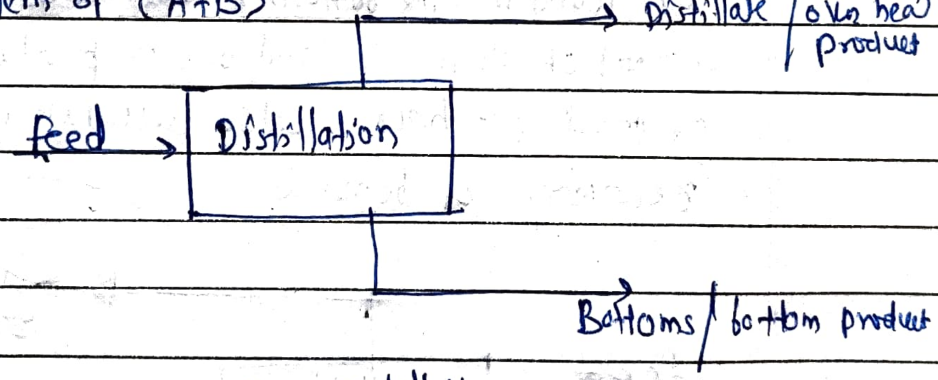


fig. Distillation

Overall material balance

$$\text{Feed} = \text{Distillate} + \text{Bottoms}$$

$$F = D + W$$

Where F is feed to a distillate column in kg & kg/h

D is the distillate in kg or kg/h. and W. bottom product in kg or kg/h.

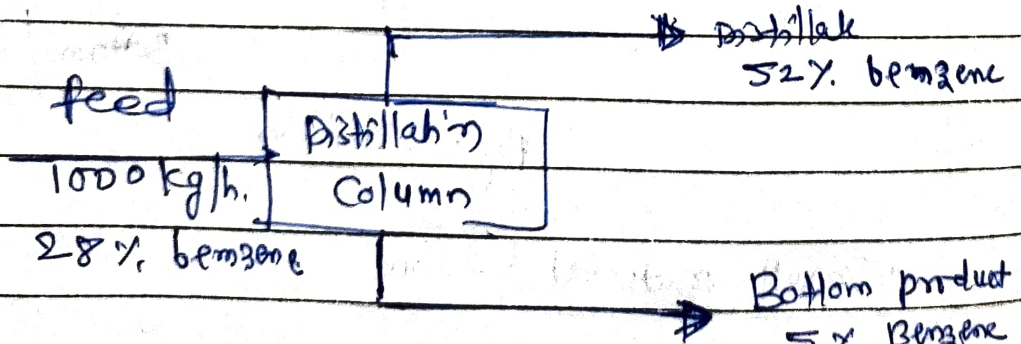
Material balance for Component

A in feed = A in distillate + A in bottom

$$x_F \cdot F = x_D \cdot D + x_W \cdot W$$

x_F, x_D and x_W are the weight fractions of A in feed, distillate and bottoms.

P. A feed Continuous fractionating column analyses by weight 28 percent benzene and 72 percent toluene. the analysis of the distillate shows 52 weight percent benzene and 5 weight % benzene was found in the bottom product. Calculate the amount of distillate and bottom product per 1000 kg of feed per hour. also calculate the percent recovery of benzene.



Overall material balance = Feed = Distillate + Bottom product

$1000 = x + y$.

$\therefore \quad x + y = 1000$

material balance of Benzene

$$x + y = 1000 \quad \text{———} \quad ①$$

material balance of benzene

Benzene in feed = Benzene in distillate + Benzene in Bottom product

$$0.28 \times 1000 = 0.52x + 0.05y$$

$$280 = 0.52x + 0.5y \quad — \quad ②$$

$$0.5y = 280 - 0.52x \quad —$$

$$y = \frac{280 - 0.52x}{0.05}$$

$$y = \frac{280}{0.05} - \frac{0.52x}{0.05}$$

$$y = 5600 - 10.4x \quad — \quad ③$$

put the value of y from eqn ③ in eqn ①

$$x + y = 1000$$

$$x + 5600 - 10.4x = 1000$$

$$x - 10.4x = 1000 - 5600$$

$$9.4x = 4600$$

$$x = \frac{4600}{9.4} = \underline{489.4 \text{ kg/hr}}$$

$$y = 1000 - 489.4 = \underline{510 \text{ kg/h}}$$

(x) Distillate flow rate = $\underline{489.4}$

(Y) Bottom product flow rate = 510.6 kg/hr

Benzen in feed = $0.28 \times 1000 = 280$ kg/hr

Benzen in distillate = $0.52 \times 489.4 = 254.49$ kg/hr

$$\% \text{ recovery of Benzene} = \frac{\text{benzene in Distillate}}{\text{benzene in feed}} \times 100$$

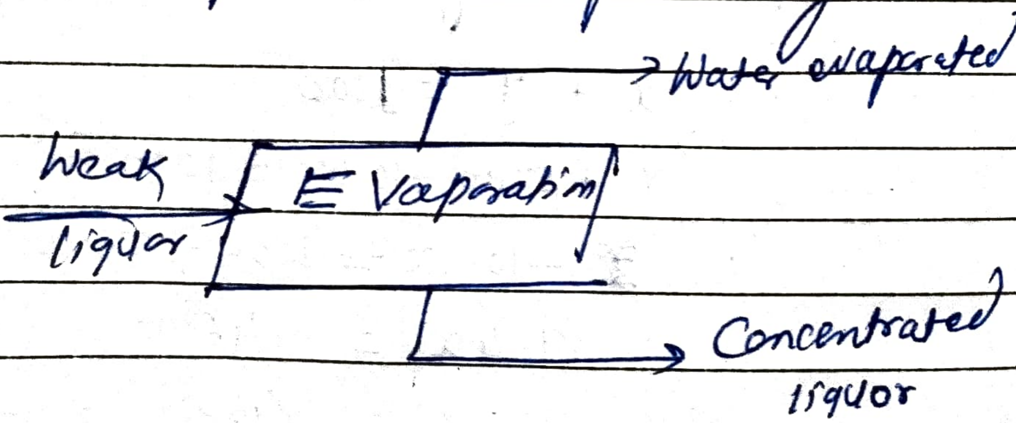
$$= \frac{254.49}{280} \times 100$$

$$= \underline{90.89}$$

Evaporation :

This operation used in a chemical industry for the concentration of weak liquor to produce a thick liquor by evaporating a portion of the solvent (generally water) by means of condensing steam.

It may be carried out in a single or multiple effect evaporation system.



Overall Material balance

Weak liquor = Water evaporated + crystallized product + Thick liquor in excess of the theoretical or

If Crystallized product is nil

Weak liquor = Water evaporated + Thick liquor

Material balance of solid (solute):

solids (solute) in Weak liquor = Solids (solute) in thick liquor

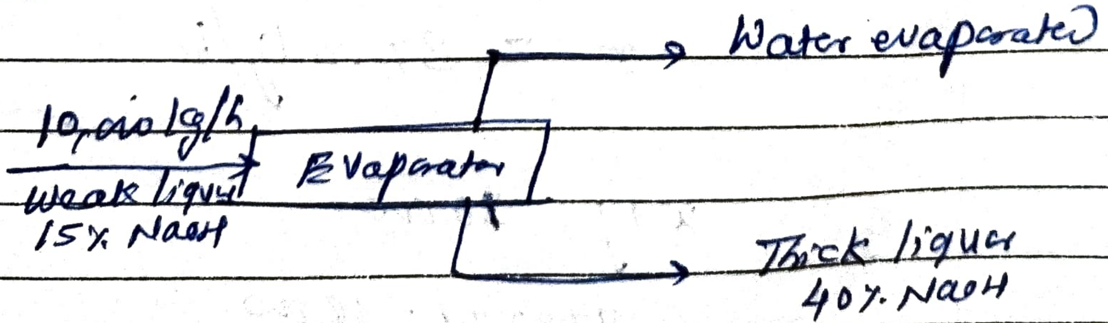
Material balance of Water

Water in Weak liquor = Water evaporated + Water in thick liquor

P. A single effect evaporator is fed with 10,000 kg/hr of weak liquor containing 15% caustic by weight and is concentrated to get thick liquor containing 40% by weight caustic NaOH

Calculate ⓐ kg/h of water evaporated
ⓑ kg/h thick liquor obtained

Soln Basis 10,000 kg/h of weak liquor



let x be the kg/h thick liquor obtained and y be the kg/h water evaporated

Overall material balance

Σ kg/h input = Σ kg per hour output

weak liquor = Thick liquor + kg/h evaporated

$10000 = x + y$

Material balance of NaOH

NaOH in the input = NaOH in the output

NaOH in weak liquor = NaOH in thick liquor

~~0.15x~~

$\frac{15}{100} \times 10000 = 0.40x$

$0.15 \times 10{,}000 = 0.40x$

$x = \frac{0.15 \times 10{,}000}{0.40}$

$x = 3750$ kg/hr

$x + y = 10{,}000$

$3750 + y = 10{,}000$

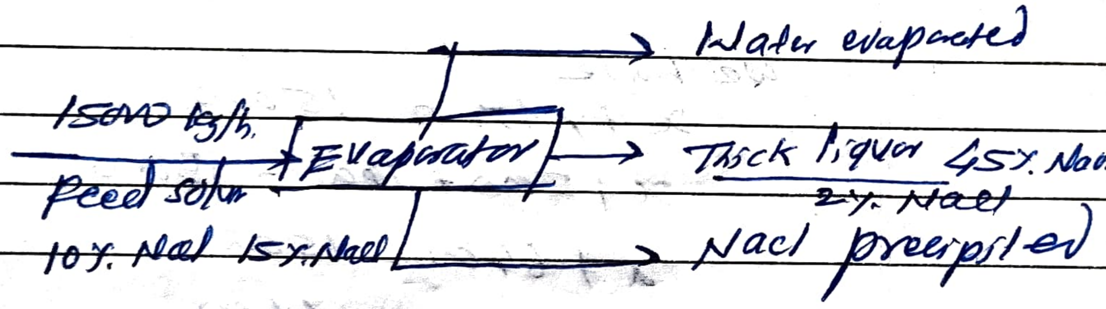
$y = 10{,}000 - 3750$

Water evaporated = 6250 kg/hr

2) An water evaporated is feed with 15000 kg/h of solution Containing 10% NaCl and 15% NaOH and rest water. In the operation. water is evaporated and NaCl is precipitated as crystals. the Thick liquor leaving the evaporator Contain 45% NaOH 2% NaCl and rest water.

Calculate ⓐ kg/h water evaporated
ⓑ kg/h. salt precipitated
ⓒ kg/h Thick liquor

Sol^n



Overall Material balance

Input = output

~~feed = Thick liquor + NaCl precip + Water evapo~~

feed = water eva + Thick liq + NaCl preps

$15000 = x + y + z$

Material balance for NaOH

NaOH in feed solution = NaOH in thick sol^n

$0.15 \times 15000 = 0.45 \times y$

$$\frac{0.15 \times 15000}{0.45} = y$$

$y = 5000$ kg/hr.

Material balance for NaCl

NaCl in feed solution = NaCl in thick liquor
+ NaCl precipitated
as a crystal

$0.10 \times 15000 = 0.02 \times 5000 + z$

$1500 = 100 + z$

$1500 - 10 = z$

1400 kg/h $= z$

We have

$x + y + z = 15000$

$x + 5000 + 1400 = 15000$

$x + 6400 = 15000$

$x = 15000 - 6400$

$x = 8600$ kg/hr

Water evaporated (x) = 8600 kg/hr

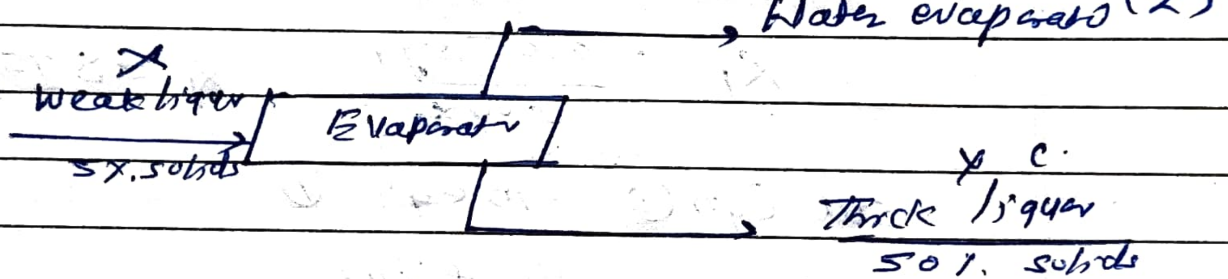
Thick liquor obtained = 5000 kg/hr

NaCl precipitated = 1400 kg/hr

3.) An evaporate system concentratating liqua 5% to 50%. solids handles 100 kg of solid per hour. If the same system is to concentrate a weak liquor from 4% to 35%. Find the capacity of system in term of solid that can be handled per hour assuming water Water evaporation capacity to be same in both the cases.

Sol^n Case I

Basis 100 kg/h of solid hadling capacity of the evaporator.



let x be the kg/h of weak liquor then we have

$$0.05x = 100$$

$$x = \frac{100}{0.05} = 2000 \text{ kg/h}$$

Let y be the kg of thick liquor then we have

$$0.5y = 100$$

$$y = \frac{100}{0.5} = 200 \text{ kg/h}$$

Overall M.B

kg of weak liquor = kg/h of thick liquor + kg/h water evaporated

2000 = 200 + water evapora

Water evaporated = 2000 − 200

Z = 1800 kg/h

Case II

1800 kg/h water evaporated

Let x_1 & y_1 be the weak liquor and thick liquor leaving evaporator

Over all M.B

$$x_1 = Y_1 + z$$

$$x_1 = y_1 + 1800 \quad — ①$$

Material balance for solid

weak liquor

$$0.04 x_1 = 0.035 y_1 \quad —$$

$$x_1 = \frac{0.035 y_1}{0.04} \quad , x_1 = 8.75 y_1 \quad — ②$$

sub. eqn ② in eqn ①

$$8.75 y_1 = y_1 + 1800$$

$$8.75 y_1 - y_1 = 1800$$

$$7.75 y_1 = 1800$$

$$y_1 = \frac{1800}{7.75} = 232.26$$

$$x_1 = y_1 + 1800$$

$$x_1 = 232.26 + 1800$$

$$= 2032.26 \text{ kg/hr}$$

Solid in weak liquor

$$= 0.04 \times 2032.26$$

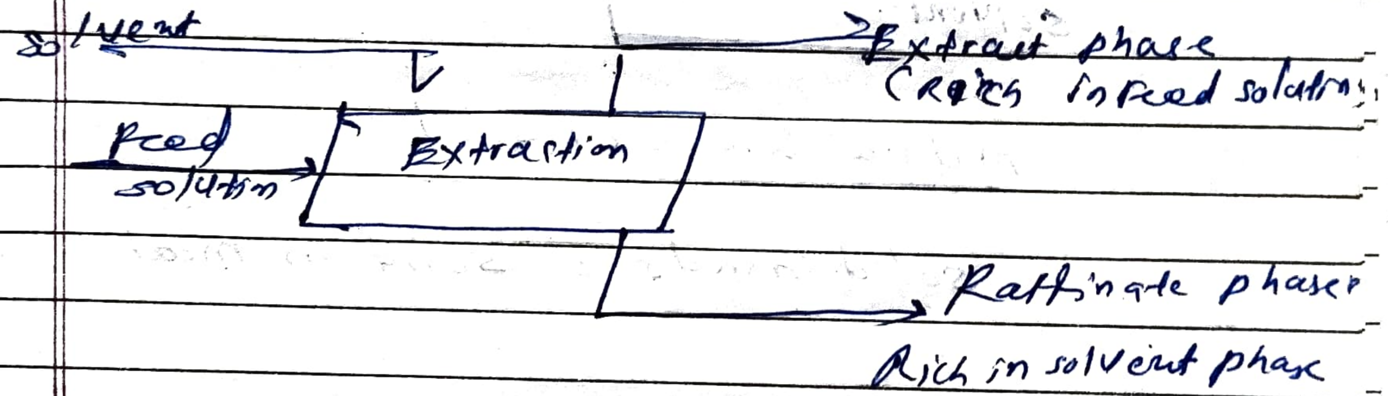
$$= 81.3 \text{ kg/hr}$$

Handling Capacity in case II = 81.3 kg/h

Extraction

This operation used in the Chemical industry for the separation of the component of liquid Mixture with help of suitable liquid solvent where in the solute from the feed solution is a Transferred in the solvent yielding the raffinate phase (rich in feed solvent) and extract phase (rich in solvent used). It is does not give a pure product and need further processing

Mixer settler, packed columns. etc



Overall M.B

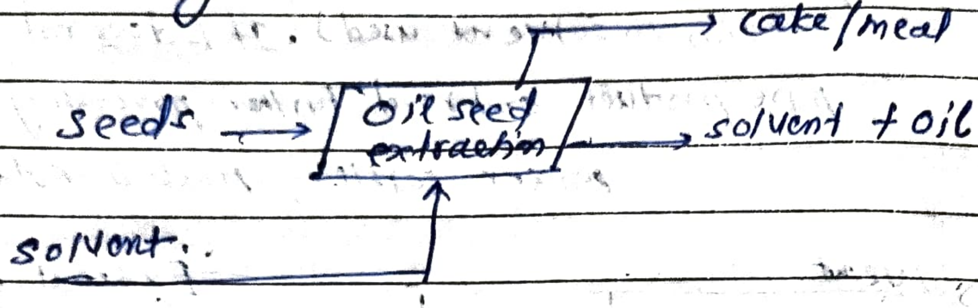
Feed solution + solvent = Extract phase + Raffinate phase

M.B. for solute

A in feed solution = A in Extract phase + A in raffinate phase

Extraction operation is also carried out for removal of a soluble constituent or solids with help of suitable liquid solvent (Here it is a solid extraction)

for example oil seed extraction or leaching of valuable metals from mineral ores.



material balance of solid

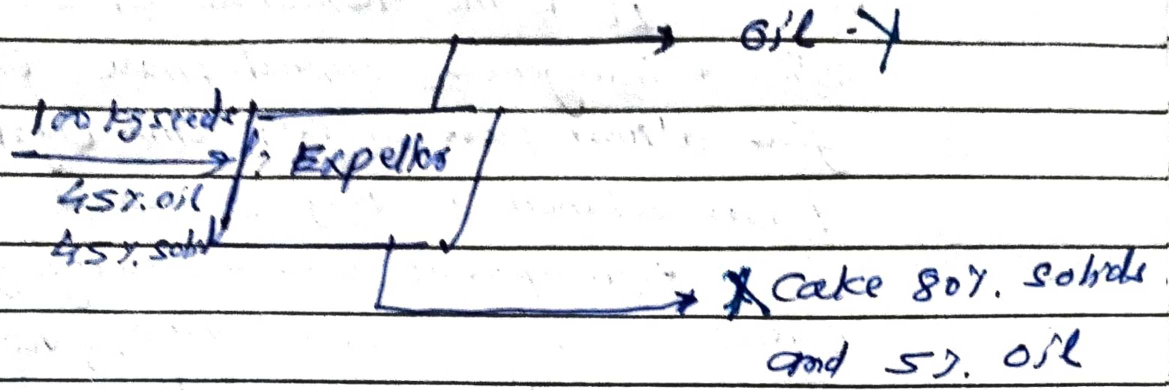
solid in seeds = solid in meal

material balance of oil

oil in seeds = oil in meal + oil in solvents (extracted oil)

Q. The ground nut seeds containing 45% oil and 45% solids are fed to expeller the cake coming out of expeller is found to contain 80% solids and 5% oil. find the % recovery of oil.

soln 100 kg of ground nut seeds.



Material balance of solids

solid in ~~cake~~ seeds = solid in cake

$0.45 \times 100 = 0.8 \times X$

$x = \frac{0.45 \times 100}{0.8} = 56.25\,kg$

cake solid = 56.25 kg.

Material balance of oil

oil in seeds = oil in cake + oil recovered

$0.45 \times 100 = 0.05 \times 56.25$ + oil recovered

$45 = 2.81$ + oil recovered

oil recovered $= 45 - 2.81$
$= 42.19$ kg

% recovery of oil $= \frac{\text{kg of oil recovered}}{\text{kg of oil seeds}} \times 100$

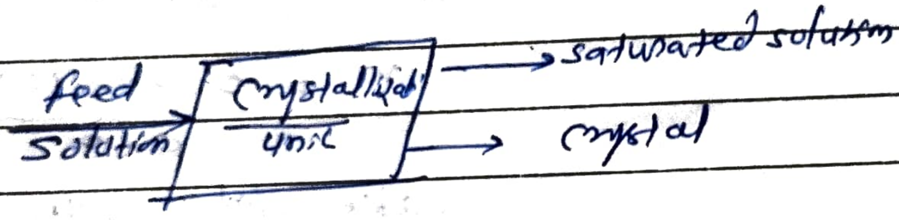
$= \frac{42.19}{45} \times 100 = 93.75$ Ans.

Crystallization :-

It is the formation of solid particles within a homogeneous liquid phase. Crystallization gives almost pure product and crystallization form solution is very Important Industrially

, equimpment used for carrying out crystallisation are sirred tank vacuum crystallizer

Crystallization of the dissolved solid from a solution is based on the difference in solubilities at different temperature. It is usually consist of concentration of solution and cooling of solution until it become supersaturation



overall material balance

feed solution = saturated solu + crystal

Material balance of solute crystals

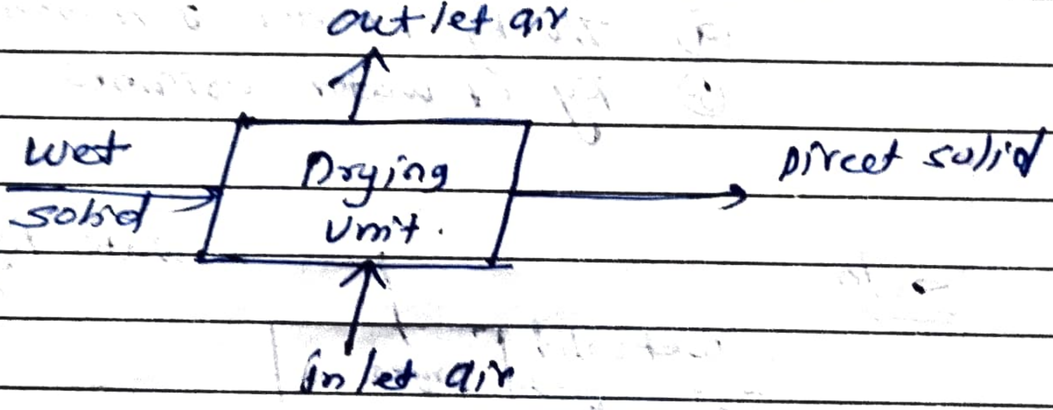
Crystal in feed solution

= Crystal obtained + crystal in saturated solution.

Drying -

This operation is carried out in the chemical Industry for the removal of a residual mixture (Water) or volatile liquid associated with wet solids with the help of hot air or inert gas (N_2) (drying medium). When the hot air is circulated over wet solids, the moisture from the solids evaporates and get added in the air is circulated over wet solid.

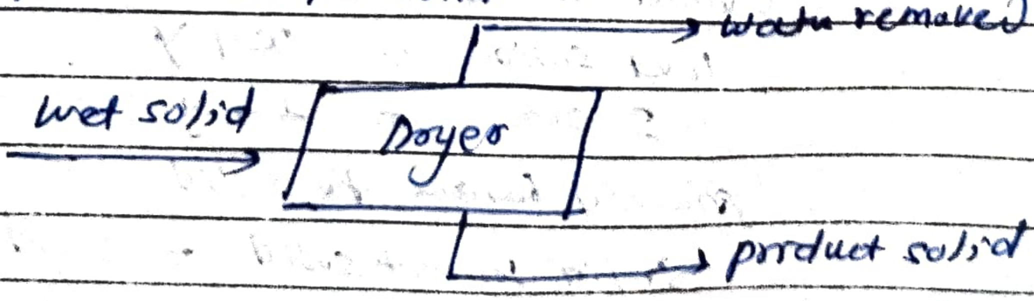
In Industry there are mainly used Tray dryer, spray dryer etc.



Material balance of Moisture

Moisture removed from solid = moisture added in air

Material balance for solid.



~~solid in wet solid~~ = solid in product

Overall material balance

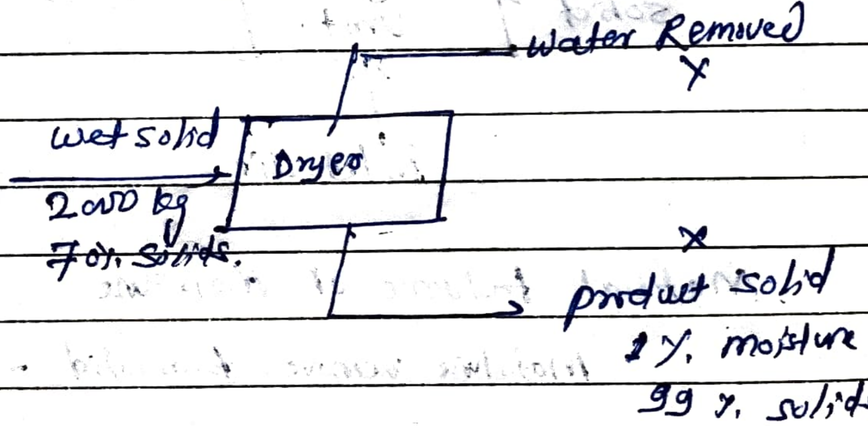
Wet solid = Water ~~evaporated~~ removed + product solids.

P→ 2000 kg of wet solids containing 70% solids by weight are fed to a tray dryer where it is a dried by hot air. the product finally obtained is found to contain 1% moisture by weight. Calculate.

ⓐ The kg of water removed from wet solid

ⓑ kg of water obtained

Soln



Overall M. B

Wet solid = $x+y$

$2000 = x+y$

Material balance for solid

Solid in wet solid = solid in product

$0.7 \times 2000 = 0.99\,X$

$$X = \frac{0.7 \times 2000}{0.99} = 1414.14 \text{ kg}$$

Over all material balance

$2000 = x + y$

$2000 = 1414.14 + y$

$y = 2000 - 1414.14$

$y = 585.86$ Kg

Water removed (y) = 585.86 kg

Kg.of · product solid = 1414.14 kg

C. 4

Material balance with chemical Reactions

completion of the reaction or vice-versa.

Definitions of Terms Involved :

Stoichiometry : It is the theory of the proportions in which chemical species combine with one another.

Stoichiometric Equation : The stoichiometric equation of a chemical reaction is the statement indicating relative moles of reactants and products that take part in the reaction. For example, the stoichiometric equation

$$CO + 2\,H_2 \rightarrow CH_3OH$$

indicates that one molecule (mol or kmol) of CO reacts with two molecules (mol or kmol) of hydrogen to produce one molecule (mol or kmol) of methanol.

Stoichiometric Coefficient : It is the number that precede the formula of each component involved in a chemical reaction.

Thus, for example, in the above cited reaction, the stoichiometric coefficient of CO is one, the stoichiometric coefficient of H_2 is two and that of methanol is one. The stoichiometric requirements of components are given as :

$$1 \text{ kmol } CO \equiv 1 \text{ kmol } CH_3OH$$

$$\equiv 2 \text{ kmol } H_2$$

Stoichiometric Ratio : It is *the ratio of stoichiometric coefficients of two molecular species/components in the balanced reaction equation.*

e.g., stoichiometric ratio of H_2 to CO is 2/1 = 2.

Stoichiometric Proportion : Two reactants, A and B, are said to be present in the stoichiometric proportion if the ratio of moles of A present to the moles of B present is equal to the stoichiometric ratio obtained from the balanced reaction equation.

Consider the following chemical reaction :

$$CO + 2H_2 \longrightarrow CH_3OH$$

For the reactants in the above reaction to be present in the stoichiometric proportion, there must be 2 moles of H_2 for every mole of CO (so that $n_{H_2}/n_{CO} = 2/1 = 2$) present in the feed to any reactor.

When the reactants are fed to a reactor in the stoichiometric proportion and the reaction goes to completion, all of the reactants are consumed. In case of the above cited reaction, for example, if 200 mol of H_2 and 100 mol of CO are initially present, the H_2 and CO would disappear at the same instant. It follows that if we start with 100 mol of CO and less than 200 mol of H_2 (i.e., if H_2 is present in less than its stoichiometric proportion) H_2 disappears before the CO_2, on the other hand, if there are more than 200 mol of H_2 initially present the CO disappears first.

Limiting Reactant / Component : *It is defined as the reactant that would disappear first if a reaction goes to completion.* It is the one which decides the extent to which a reaction can proceed. The limiting reactant is always present in less than its stoichiometric proportion relative to the other reacting components. It is the reactant which is present in the smallest stoichiometric amount, i.e., the reactant which is not present in excess of that required to combine with any of the other reactants.

It is the reactant which is present in such proportions that its consumption/disappearance by the reaction will limit the extent to which the reaction can proceed (i.e., the extent of reaction).

Excess Reactant : It is defined as the reactant which is in excess of the theoretical or stoichiometric requirement as determined by the desired reaction. The excess component / reactant always found in the product stream though the reaction proceeds to completion.

For example, consider the following reaction :

$$C_2H_4 + \frac{1}{2} O_2 \rightarrow C_2H_4O$$

4.2

4.4

In industrial practice of producing ethylene oxide by oxidation of ethylene, oxygen/air fed to the reactor is always in excess of that theoretically required. Thus, ethylene is the limiting reactant and oxygen/air is the excess reactant.

It is a reactant present in excess of the limiting reactant.

When all reactants are present in the stoichiometric proportion, then none of the reactants involved is limiting.

For example, $N_2 + 3\,H_2 \rightarrow 2\,NH_3$

N_2 and H_2 are always fed to reactor in their stoichiometric proportion i.e. 1 mole N_2 to 3 moles H_2 so no reactant is limiting.

Percent Excess : The excess reactant involved in the reaction is generally specified in terms of percent excess. It is the amount in excess of the stoichiometric (theoretical) requirement expressed as a percentage of the stoichiometric/theoretical requirement.

Consider the reaction : A + B → C

wherein B is the excess reactant. Then

$$\boxed{\therefore \left[\begin{array}{l}\text{Percent}\\ \text{excess of B}\end{array}\right] = \left[\frac{\begin{array}{l}\text{moles of B}\\ \text{supplied}\\ \text{or fed}\end{array} - \begin{array}{l}\text{moles of B}\\ \text{theoretically}\\ \text{required}\end{array}}{\begin{array}{l}\text{moles of B}\\ \text{theoretically}\\ \text{required}\end{array}}\right] \times 100} \quad \text{... (4.1)}$$

Moles of B theoretically required are the moles of B that would correspond to stoichiometric proportion and are calculated based on limiting reactant charged.

Equation (4.1) is also valid on weight basis.

The above equation can be rearranged to calculate the quantity of the excess reactant actually supplied.

$$\boxed{\left[\begin{array}{l}\text{moles of B}\\ \text{actually fed}\\ \text{or supplied}\end{array}\right] = \left[\begin{array}{l}\text{Stoichiometric}\\ \text{requirement or}\\ \text{theoretical}\\ \text{requirement of B}\end{array}\right]\left(1 + \frac{\%\ \text{excess B}}{100}\right)} \quad \text{... (4.2)}$$

The quantity of excess reactant must be found based on the quantity of limiting reactant fed to the reactor.

Consider, for example, the reaction

$$SO_2 + \frac{1}{2} O_2 \longrightarrow SO_3$$

and suppose that 100 mol SO_2/h and 75 mol O_2/h are fed to a reactor. SO_2 is clearly the limiting reactant, and to be in stoichiometric proportion, moles of O_2 would have to be 50 mol/h. The percent excess of O_2 is therefore

$$\%\ \text{excess}\ O_2 = \left(\frac{75 - 50}{50}\right) \times 100 = 50$$

Conversion : The conversion is always based on the limiting reactant and it gives idea
garding the degree of completion of a reaction. The unreacted quantities of raw materials
e easily obtained knowing the charged quantities with the help of conversion. This, in turn,
ves us idea regarding whether recycling is to be done or not for the process to be
onomically feasible.

Conversion is the fraction of some key reactant that is converted into products.

Consider the chemical reaction :

$$A + B \rightarrow C$$

ere A is the limiting reactant and B is the excess reactant. Then,

The conversion or fractional conversion of A is the ratio of the amount of A reacted to amount of A charged or fed to the reactor. The percentage conversion of A is the amount reacted expressed as a percentage of the amount of A charged or fed to the reactor.

The amount of A can be expressed on mole or weight basis. If amount of A is expressed
oles then

$$\boxed{\%\text{ conversion of 'A'} = \frac{\text{moles (or mass) of A reacted}}{\text{moles (or mass) of 'A' charged or fed}} \times 100}$$

n case of recycle operations, the term namely per pass conversion is commonly used. per pass conversion is defined as the *quantity of limiting reactant reacted/consumed essed as the percentage of the limiting reactant in the mixed feed.*

f 100 mol of reactant A are fed and 75 of them react, the fractional conversion is 0.75 ercentage conversion is 75%) and the fraction unreacted is 0.25. If 50 mol of reactant A d and the percentage conversion is 80%, then (0.80) (50) = 40 mol of reactant A are d and (0.20) (50) = 10 mol of A remain unreacted.

egree of completion of a reaction is expressed as the percentage of the limiting reactant rted into the product.

ield and Selectivity : In most of the chemical processes, though the objective is to e a desired product, the raw materials may also undergo a series of parallel reactions eactions) resulting into production of undesired materials which has reverse effect on onomics of the process. In such cases (in industrial practice), the steps are taken to s the side reactions by use of selective catalyst, addition of inhibitors in the feed, etc.

e terms yield and selectivity are used in case of multiple reactions to give the ation regarding the degree to which the desired reaction predominates over the side n (or reactions) involved.

nsider the reactions :

$$A + B \rightarrow C$$

$$C + B \rightarrow D$$

$$A \rightarrow C \rightarrow D \quad \text{... (reactions in series)}$$

$$A \rightarrow C$$

$$A \rightarrow D \quad \text{... (parallel reactions)}$$

C is the desired product, D is the undesired product and A is the limiting reactant. the yield of 'C' is given as :

$$\boxed{\text{Yield of C} = \frac{\text{moles of A reacted to produce C}}{\text{moles of A totally reacted}} \times 100}$$

ield of the desired product is the quantity of the limiting reactant reacted to produce it ssed as the percentage of the quantity of the limiting reactant reacted totally (i.e. by all ons).

electivity is the ratio of the moles of the desired product produced to the moles of the sired product (by-product) produced.

onsider the parallel reactions :

→ C and A → D, where C is the desired product and D is the undesired product, in ase, selectivity is given as :

$$\boxed{\text{Selectivity of C relative to D} = \frac{\text{moles of C (desired product) formed}}{\text{moles of D (undesired product) formed}}}$$

electivity is also defined as the ratio of the amount of the limiting reactant reacted to the ed product to the amount of it reacted to produce the undesired product. If yield is then the selectivity is 1.

C-4

Material balances with chemical Reaction

1) The Carbon monoxide is reacted with hydrogen to produce methanol. calculate from the reaction

a) stoichiometric ratio H_2 TO CO

b) K mol of CH_3OH produced per Kmol CO reacted

c) weight ratio of CO to H_2 if both are fed to reactor in a Stoichiometric proportion

d) The quantity of CO required to produce 100 kg of CH_3OH.

soln

$$CO + 2H_2 \rightarrow CH_3OH$$

Sotoichiometric Co. efficient

$CO = a = 1$

$H_2 = b = 2$

a) Stoichimetric ration H_2 to CO

$$\frac{b}{a} = \frac{2}{1} = 2 \quad \text{Ans}$$

b) Co. reacted to produce CH_3OH

$$= \frac{1}{1} = 1$$

c) weigth ratio CO to H_2

CO used in kg

$\therefore$ Moles = $\frac{\text{weight of substance}}{\text{molecular weight}}$

$$1 = \frac{\text{weight of sub. (CO)}}{28}$$

$28 \times 1 =$ weight of sub.

28 kg = CO used. to fed

H_2 fed to reactor in kg

$$\text{moles} = \frac{\text{weigth of } H_2}{\text{mol. weigth}}$$

$$2 = \frac{\text{weight of } H_2}{2}$$

$$4 = \text{weight of } H_2$$

weigth ratio

$$= \frac{28}{4} = 7$$

d) The quantity CO required to produce 1000 kg of CH_3OH

28 kg required to produce 32 kg CH_3OH

for 1000 kg CH_3OH produced ?

$$= \frac{32}{28} \times \frac{1000}{1} = 875 \text{ kg}$$ ans

2) Ammonia is produced by following reaction

$N_2 + 3H_2 \longrightarrow 2NH_3$

Calculate ⓐ molal flow rate of hydrogen corresponding to nitrogen feed rate of 25 kmol/h if they are fed in stoichiometric proportion

b) The kg of ammonia produced per hour % conversion is 25 and nitrogen feed rate is 25 kmol/h.

Soln

$N_2 + 3H_2 \longrightarrow 2NH_3$

Stoichiometric proportion of N_2 to H_2 from the Reaction is 1 : 3.

- Molal flow rate of Hydrogen in stoichiometric proportion

$= \frac{3}{1} \times 25 = 75$ kmol/h

- moles of N_2 reacted = kmole of N_2 fed per hour ~~% conversion of NH_3~~ × % conversion of N_2

$= 25 \times \frac{25}{100}$

$= 6.25$ kmol/h

- 1 kmol of N_2 produced 2 kmol of NH_3

NH_3 produced with 1 kmol N_2 reacted $= 2 \times 6.25$

$= 12.50$ kmol/h

Amount of NH_3 produced = NH_3 produced × mol. weight

= 12.50 × 17

= 212.5 kg/hr

③ In a production of Sulphur trioxide, 100 kmol of SO_2 and 200 kmol of O_2 are fed to a reactor. the product stream is found to contain 80 kmol SO_3. Find the % conversion of SO_2.

Reaction

$$SO_2 + \frac{1}{2}O_2 \rightarrow SO_3$$

1 kmol SO_3 produce to required 1 kmol SO_2

80 kmol of SO_3 ⟶ ?

SO_2 reacted = $\frac{80}{1} \times 1$ = 80 kmol

$$\% \text{ Conversion of } SO_2 = \frac{\text{kmol of } SO_2 \text{ reacted}}{\text{kmol of } SO_2 \text{ charged}} \times 100$$

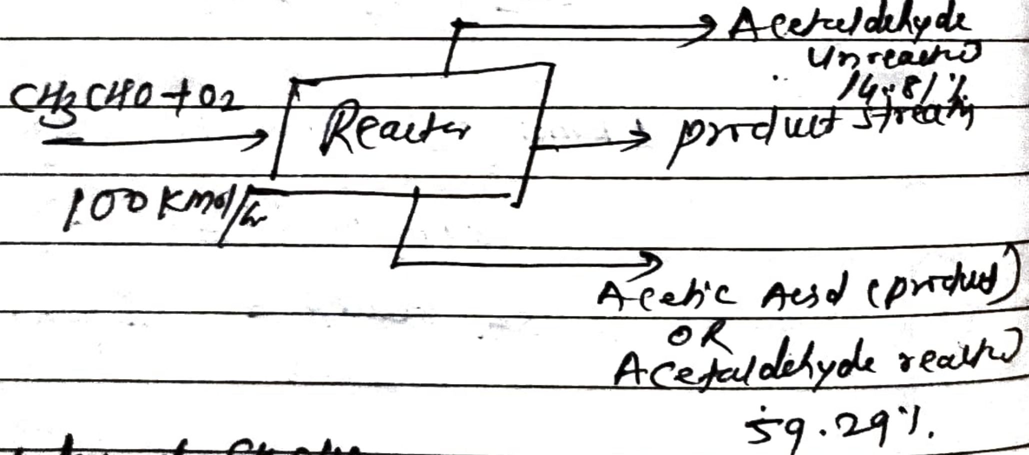
$$= \frac{80}{100} \times 100 = 80$$

4) In Manufacture of acetic acid by oxidation of acetaldehyde 100 kmol of acetaldehyde is fed to reactor per hour. The product leaving the reactor contain 14.81% acetaldehyde. 59.26% acetic acid, and rest oxygen (on mole basis) Find the % conversion of acetaldehyde.

Soln 100 kmol/h acetaldehyde charged to reactor

Reaction

$$CH_3CHO + O_2 \longrightarrow CH_3COOH$$



M. balance of CH_3CHO

CH_3CHO feed To Reactor = Acetaldehyde reacted + CH_3CHO unreacted

$$100 = 0.5929x + 0.1481x$$

$$100 = 0.741x$$

$$\frac{100}{0.741} = x$$

$$x = 134.95 = 135$$

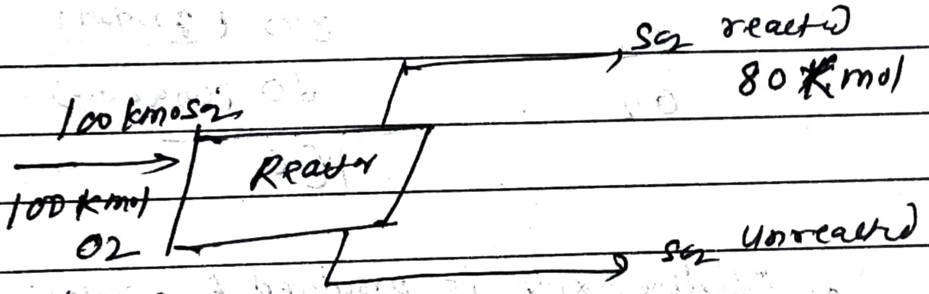
∴ Acetaldehyde reacted = 0.5929(135)
= 80.01 kmol/hr

% conversion of acetaldehyde

$$= \frac{\text{Acetaldehyde reacted}}{\text{acetaldehyde charged}} \times 100$$

$$= \frac{80}{100} \times 100 = \underline{\underline{80}}$$

⑤ A production of sulphur tri oxide, 100 kmol of SO_2 and 100 kmol of O_2 are fed to reactor If % Conversion of SO_2 is 80.. calculate the composition of the product stream on mole basis.



Material balance of SO_2

SO_2 charged to reactor = SO_2 reacted + SO_2 unreacted

100 = 80 + SO_2 unreacted

SO_2 unreacted = 100 − 80
= 20 kmol

1 m kmol of SO_2 = 1 kmol SO_3

80 kmol of SO_2 reacted = 80 kmole of SO_3 produced

Similarly

from reaction 1 kmol SO_2 reacted $= (\frac{1}{2})\,0.5$ kmol of O_2 reacted

∴ 80 kmol SO_2 reacted and $\frac{1}{2}$ kmol of O_2 reacted

means half of the SO_2

$\frac{1}{2} \times 80 = 40$ Kmol

Material balance of O_2

O_2 charged = O_2 reacted + O_2 unreacted

100 = 40 + O_2 unreacted

~~O_2 char~~

100 − 40 = O_2 unreacted

60 = O_2 unreacted

O_2 reacted = 60 kmol

Composition of product stream

Component	Quantity kmol	mol %
SO_2	20 (unreacted)	$20/160 \times 100 = 12.5$
SO_3	80 (product)	$80/160 \times 100 = 50$
O_2	60 (unreacted)	$60/160 \times 100 = 37.5$
	160	100

P-6. Ethylene oxide is produced by oxidation of ethylene. 100 kmol of ethylene are fed to reactor and product is found to contain 80 kmol ethylene oxide and 10 kmol of CO_2. Calculate

a) the % conversion of ethylene

b) % yield of ethylene oxide

Soln 100 kmol of ethylene fed to reactor

Ethylene, O_2 → Reactor → product C_2H_4O, C_2H_4, CO etc

Reaction I

$$C_2H_4 + \frac{1}{2}O_2 \rightarrow C_2H_4O$$

Reaction II

$$C_2H_4 + 3O_2 \rightarrow 2CO_2 + 2H_2O$$

f R. 1

80 kmol of ethylene oxide produce means 80 kmol of C_2H_4 reacted

from Reaction II

1 kmole of C_2H_4 reacted and 2 kmole of CO_2 produced

∴ 10 kmol of CO_2 produced mean 5 kmol of C_2H_4 reacted

∴ C_2H_4 totally reacted from Reaction I & Reaction II

C_2H_4 totally reacted = C_2H_4 reacted Reaction I + Reaction II

$$= 80 + 5$$

$$= 85$$

$$\% \text{ conversion of } C_2H_4 = \frac{C_2H_4 \text{ reacted}}{C_2H_4 \text{ fed}} \times 100$$

$$= \frac{85}{100} \times 100 = 85\,\%$$

$$\therefore \text{yield of } C_2H_4O = \left(\frac{\text{kmole of } C_2H_4 \text{ reacted to produce } C_2H_4O}{\text{kmol } C_2H_4 \text{ totally reacted}} \right) \times 100$$

$$= \frac{80}{85} \times 100$$

$$= \underline{\underline{94.12}}\ \%$$