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Process Calculations

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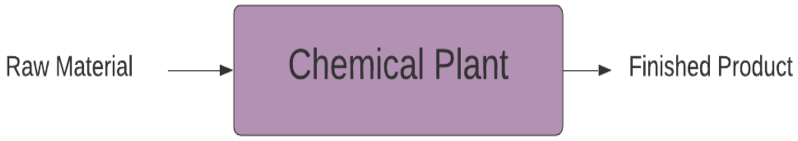
Lecture-01

Introduction of Chemical Engineering or Process engineering

Chemical Engineering is all about converting raw material to finished product at very large scale or industrial scale. Chemical engineer is one who applies and uses principles of chemical engineering in any of its various practical applications

- Design, manufacture, and operation of plants and machinery in industrial chemical and related processes
- Development of new or adapted substances for products ranging from foods and beverages to cosmetics to cleaners to pharmaceutical ingredients, petrochemical ,oil refining are among many other products
- Development of new technologies to make plants cost effective and eco friendly.



Chemical engineering- plants ccale or industrial scale with focus on large scale production.
Chemistry- Lab scale for small scale with focus on research and development.

Let's take some examples of some typical chemical plants to understand overview of chemical engg.

1) Sugar industry

In sugar industries solid sugar in granular form is produced from sugarcane. Schematic line diagram is given in figure 1.1.Sugarcane will be first crushed and compressed into the Crusher to extract sugarcane juice. This juice is sent to the evaporator for concentrating it by vaporization.Thick liquor is sent to the crystallizer where sugar crystals will be formed. The liquid and sugar crystal will be separated by using a centrifuge, remaining liquid is known as molasses and it can be used as raw material for production of ethyl alcohol. For this purpose molasses will be send to a fermentor in which biochemical reaction will happen and ethyl alcohol will be form and finally ethyl alcohol is separated in a distillation column so we are getting ethyl alcohol and solid sugar crystals as finished products from sugarcane.

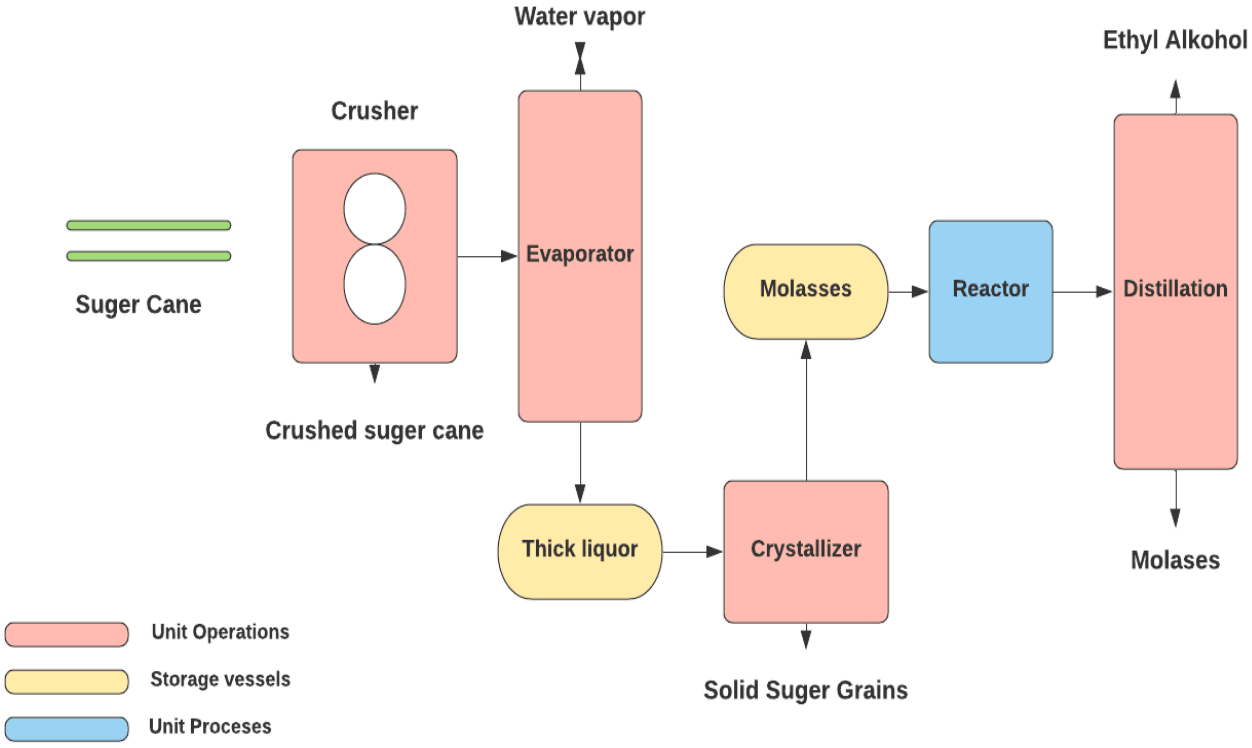


Fig: 1.1, Line diagram of suger industry

All the units of sugar industry can be divided into divided into two parts

1. Unit operation- Only Physical changes. No chemical Reaction
2. Unit processes- Chemical changes or Chemical reaction

Unit operation

- Crusher
- Evaporator
- Crystalizer
- Distillation

Unit Process

- Fermenter

2) Crude Oil Refinery

In oil refineries numeros product's like LPG, gasoline, Petrol, diesel and aviation fuel are produced by the processing of crude oil. Firstly crude-oil will be treated into a distillation column where different components of crude oil will be separated on the basis of their boiling points. further these products will be treated as in various units for converting it into a finished product..

Chemical Plant

1. raw material first will be treated through various unit operations so that it can be conditioned or can be made ready for chemical conversion (Chemical Reaction).
2. Next step is the unit process, in this step a chemical reaction will happen in to a reactor. Output of unit process will contain reactants, desired products and byproducts also.
3. finally unreacted and by products will be separated from desired products using various unit operations.

Fig:1.2, Chemical PLant

Process calculation

process calculation uses the principle of material and energy balance to find raw material requirement and energy requirement for given plant production capacity.

GATE syllabus process calculation

- mass and energy balance
- Tie Component
- Recycle
- bypass
- Purge

Syllabus will be covered in following parts

- Basic concept
- mass and energy balance for unit operation
- mass and energy balance for unit process
- Combustion

Lecture-02

Ideal gas

- The molecules in a gas can be considered small hard spares.
- all collisions between gas molecules are elastic and all motions is frictionless.
- distance between molecules on an average is much larger than the size of the molecules.
- the gas molecules are constantly moving in random direction with a distribution of speed.
- there is no attraction or repulsive forces between molecules as well as the surrounding

Boyle's law

$P \propto (1/V)$: T is constant ⇒ $V \propto (1/P)$:T is constant

Charles law

$V \propto T$: P is constant

Avogadro's law

the number of molecules per unit volume is same for all gases to a fixed temperature and pressure

- The number of molecules in 22.4 litres of any gas is 6.022 x 1023 . This number is called Avogadro number
- 22.4 litre is volume of one mole gas at STP (273 K and 1 atm pressure)
- $V \propto n$ (number of moles of gases) at constant T & P.

Ideal gas law

$V \propto (1/P)$	Boyle's law
$V \propto T$	Charles law
$V \propto n$	Avogadro's law

Hence,

$$V \propto \frac{nT}{P} \quad \Rightarrow \quad PV \propto nT$$

$$\Rightarrow \quad PV = nRT$$

R= universal gas constant

Dalton's law

Total pressure of a mixture of ideal gases is the sum of the partial pressures of individual gases.

suppose a mixture of gases contains $n_1 n_2, n_3$,........ moles of different gases
using ideal gas law
$PV= (n_1+n_2+n_3+.......) RT$
$PV= n_1RT+n_2RT+n_3RT+.......$
$P= (n_1RT/V)+(n_2RT/V)+(n_3RT/V)+..........$
$P=P_1+P_2+P_3+........$

STP :(standard temperature and pressure)= 0 ℃and 1 atm
NTP:(Normal temperature and pressure)= 20 ℃ and 1 atm
R= 8.314 if all units are in IS units

Density of Ideal Gas

$PV= nRT$
$PV= wRT/M$ (w= weight in grams, M= molecular weight)
$\rho=w/V=PM/RT$

Units of pressure

One atmospheric pressure or 1 atm
$= 101.32x10^5$ N/m^2 or Pascal
=10.33 meter of water column
=76 cm of Hg column
=1.013 bar
=760 torr

Example-01

An O_2 cylinder volume 30 litre has initial pressure 15 ATM and at 27 degree centigrade. after some O_2 is withdrawn from the cylinder the gauge Pressure drops to 11 atm temperature 17 degree centigrade. Estimate the oxygen taken out of the cylinder ?

Solution
Using ideal gas law
$PV= nRT$
for initial condition $P_1 V_1= P_2 V_2$
$(15 x1.013x 10^5) x (30 x 10^{-3})= n_1 x 8.314 x 300$
initial number of moles of oxygen $n_1=18.28$

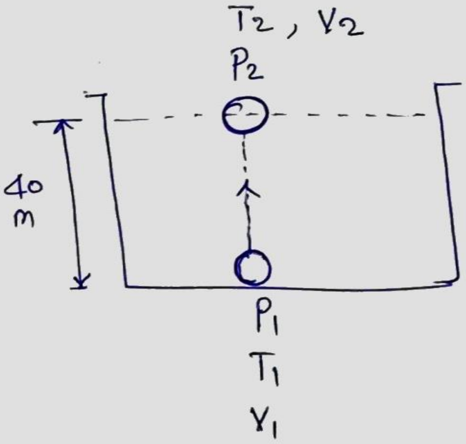
After removing some oxygen from cylinder n_2 moles of oxygen remains
Applying ideal gas law $PV= nRT$
$(11 x1.013x 10^5) x (30 x 10^{-3})= n_2 x 8.314 x 290$
Final number of moles of oxygen $n_2= 13.867$

Number of moles of oxygen removed = n_1-n_2 = 4.41
Weight of oxygen removed= 32 x 4.41 = 141.19 gm

Example-02

an air bubble of volume 1 cm cube risen from bottom of a lake 40 metre deep at temperature of 12 degree centigrade to what volume does it grow when it reaches the surface which is at temperature of 35 degree centigrade

Solution



$P_1 = P_{atm} + \rho g h_1$

$P_1 = 1.013 \times 10^5 + 1000 \times 9.81 \times 40$

$P_1 = 4.937 \times 10^5$

$P_2 = 1.013 \times 10^5$

$T_1 = 12°C = 285 °K$

$T_2 = 35°C = 308 \ K$

$V_1 = 1.0 \ cm^3$

using idel gas law —

$$P_1 V_1 = nRT_1$$
$$P_2 V_2 = nRT_2$$

$$\frac{P_1}{P_2} \cdot \frac{V_1}{V_2} = \frac{T_1}{T_2} \Rightarrow \frac{V_2}{V_1} = \frac{P_1 T_2}{P_2 T_1}$$

$$\frac{V_2}{V_1} = \frac{4.937}{1.013} \times \frac{308}{285} \Rightarrow V_2 = 5.266 \ V_1$$

$$V_2 = 5.266 \ cm^3$$

Lecture - 03 / ~~Laws of Conservation~~ Solution

Concentration :- Liquid

Molarity = g moles of solute / volume of solution

Molality = g moles of solute / Kg of solvent

Normality = gram equivalent / volume of solution

Mass Concentration = $\frac{\text{mass of solute}}{\text{Volume of solution}}$

gram equivalent = $\frac{\text{mass in gram}}{\text{equivalent weight}}$

Equivalent weight = $\frac{\text{Molecular wt}}{\text{Valancy}}$

Valancy = No of electron transfer during chemical reaction

$CaCO_3$ = 2

NaCl ~~Na_2CO_3~~ = 1

$$\boxed{N = M \times V}$$

$$\boxed{\text{Normality} = \text{Molarity} * \text{valancy}}$$

$$\boxed{N_1V_1 = N_2V_2}$$

Concentration of gases & solids :-

x_{mass} = Mass fraction = $\frac{m_a}{m_a + m_b}$

m_a = mass of A

m_b = mass of B

x_{mole} = Mole fraction = $\frac{\text{moles of A}}{\text{moles of A + moles of B}}$

Mass ratio = $\frac{m_a}{m_b}$

mole ratio = $\frac{\text{moles of A}}{\text{moles of B}}$

* Concentration of gases can be represen~~tatitte~~ted by partial pressure

p_a , p_b

mole ratio $\frac{A}{B} = \frac{p_a}{p_b}$

mole fraction = $\frac{p_a}{p_a + p_b}$

Eexample :-

A solution of 20% (by weight) NaOH is having density of 1.196 Kg/lit. Express concentration in terms of Molarity, Molality & Normality.

basis : 100 gm solution

20 gm NaOH, 80 gm water

$$\text{Volume of solution} = \frac{0.1}{1.196} \text{ lit}$$

$$= 0.0836 \text{ lit}$$

$$\text{Moles of NaOH} = \frac{\text{gm of NaOH}}{\text{Molecular weigh}}$$

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

$$\text{Molarity} = \frac{\text{moles of NaOH}}{\text{Volume of solution}} = \frac{0.5}{0.0836} = 5.98 \text{ M}$$

$$N = \upsilon \times M$$

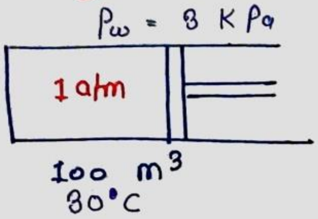
$$\text{Normality} = 1 \times 5.98 = 5.98 \text{ N}$$

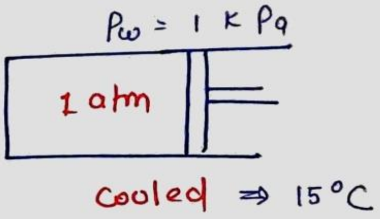
$$\text{Molality} = \frac{\text{moles of NaOH}}{\text{Kg of } H_2O} = \frac{0.5}{0.08}$$

$$= 6.25$$

Example :-

moist air is cooled at constant pressure 1 atm in piston device. initial partial pressure of of water vapor [redacted] 3.00 kPa and final 1 kPa. find kg of water condensed.





Initial condition $pV = nRT \Rightarrow n = \frac{PV}{RT}$

$$n = \frac{1.0132 \times 10^5 \times 100}{8.314 \times 303} = 4022.00$$

$$\text{moler fraction of water} = \frac{p_w}{p_t}$$

$$= \frac{3 \times 10^3}{101.32 \times 10^3}$$

$$\text{moles of water initially} = \frac{4022 \times 3}{101.32}$$

$$= 119.088 \text{ moles}$$

$$\text{kg of water vapor} = \frac{119.088 \times 18}{1000} = 2.143$$

final condition

$$\text{moler fraction of water vapor} = \frac{p_a}{p_t}$$

$$= \frac{1 \times 10^3}{101.32 \times 10^3}$$

$$= 9.8697 \times 10^{-3}$$

air present = 4022 − 119.088 = 3902.91 moles

n_w = moles of water

$$\frac{n_w}{n_w + 3902.91} = 9.8697 \times 10^{-3}$$

$101.32\, n_w = n_w + 3902.91$

$n_w = 38.90$ moles

$n_w = 0.70028$ Kg

Change in water content = water condensed

= 2.143 − 0.70028

= 1.4427 Kg

Example :-

400 ml of H_2SO_4 has density 1.08 g/ml

Calculate molarity of solution — (H_2SO_4 is 20% by ~~volume~~ weight)

density = 1.08 gm/cm

mass of solution = 1.08 × 400 = 432 gm

H_2SO_4 is = 0.2 × 432 = 86.2 gm

moles of H_2SO_4 = $\frac{86.2}{98}$ = 0.8795

$$\text{molarity} = \frac{\text{moles of } H_2SO_4}{\text{Volume of solution in lit}} = \frac{0.8795}{0.4}$$

= 2.198 M

Solubility :-

as we increase the concentration of solute. solution will reach @ equillibrium called saturated solution. any further increase of solute will lead to emmicibility or crystilization. concentration of saturated solution is called solubility.

it can be $= \frac{\text{mole}}{\text{lit}}$

or $= \frac{\text{mole}}{\text{kg of solution}}$

or any other unit of concentration

T ↑
solubility ↑

Example :-

A saturated solution at 80°C contains 5 mole of solute (mole wt = 50 kg / k mole) per kg of solvent the solubility at 100°C is 10 mole of solute per kg of the solvent. if 10 kg of the original solution is heated to 100°C, then the weight of additional solute that can be dissolved in it, is ?

take 10 kg of solution

let x kg solute , (10 − x) kg solvent

initially

$$5 \frac{\text{mole of solute}}{\text{kg of solvent}} = \frac{x / 50 \times 10^{-3}}{(10 - x)}$$

$0.25(10-x) = x \Rightarrow x = 2$ kg

initially 8 kg solvent
2 kg solute }

Now heated to 100 °C and y kg solute added to make this saturated solution.

$$10 = \frac{(2+y)}{50\times10^{-3}} \Big/ 8$$

$y = 2$ kg

Que: The molar composition of a gas is 10% H_2, 10% O_2, 80% CO_2 and balance is H_2O, If 50% H_2O condenses, the final mole % of H_2 in the gas on a dry basis will be & wet basis

bases :-

100 mole of gas contains

10 mole H_2
10 mole O_2
80 mole CO_2
50 mole H_2O

wet basis :-

50% H_2O condensed = $50 \times 0.5 = 25$ mole condensed

now $H_2 = 10$ mole $O_2 = 10$ mole
$CO_2 = 30$ mole $H_2O = 25$ mole

$$\% \text{ of } H_2 = \frac{10}{10 + 10 + 30 + 25} \times 100$$

$$\% \text{ of } H_2 = 13.33 \%$$

<u>Wet basis</u> composition of H_2 = 13.33%

⇒ Dry basis — H_2O will be removed from components —

10 mole H_2
10 mole O_2
30 mole CO_2

$$\% H_2 = \frac{10}{10 + 10 + 30} \times 100$$

$$= 20 \%$$

Lec-4/Fundamental Principle of Mass & Energy conservation

* Mass & Energy of isolated system can not be destroyed or created by any physical or Chemical transformations.

Material and energy balance for unit operation and unit process :—

universe can be assumed as an isolated system

$$\left.\begin{array}{l} E_{unit} + E_{universe} = \text{constant} \\ M_{unit} + M_{universe} = \text{constant} \end{array}\right\} \text{conservation of mass \& Energy}$$

material balance —

$$\Delta M_{unit} + \Delta M_{universe} = 0$$

$$\Delta M_{unit} + M_{out} - M_{in} = 0$$

$$\Delta M_{unit} = M_{in} - M_{out}$$

accumulation = in - out

for continuous process :—

$$\boxed{\text{rrate of accumulation mass} = \dot{m}_{in} - \dot{m}_{out}}$$

similarily

$$\boxed{\text{rrat of accumulation of energy} = \dot{E}_{in} - \dot{E}_{out}}$$

unit operations :—

- Gas Absorption
- Distillation
- Leaching
- Extraction
- Drying
- adjorption
- crystalization
- evaporation

} physical changes

Mechanical operations

- screening
- size reduction
- sedimentation
- centrifuge
- Classifier

} mechanical Change

Unit processes :—

- Reactor
- Fermentor

} chemical changes

gas Absorption :—

Any unit operation can be batch or continuous operation.

Steady State ~~process~~ operation :—

In steady state operation, all process parameters will be constant with respect to time. most continuous operations are steady state operation @ Industrial scale.

Unsteady State operation :—

Condition with in the system (process parameter P, T, ρ, C) will change with respect to time. often batch operations are unsteady state operations.

Material balance —

rate of accumulation = in – out

for steady state operation

accumulation = 0

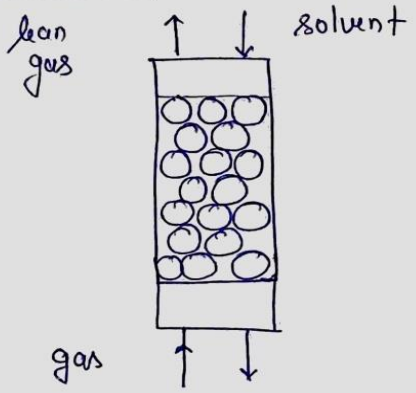
hence in − out = 0

$\boxed{\text{rate of in = rate of out}}$ steady

for unsteady operations :—

$\boxed{\text{rate of accumulation = rate in — rate out}}$

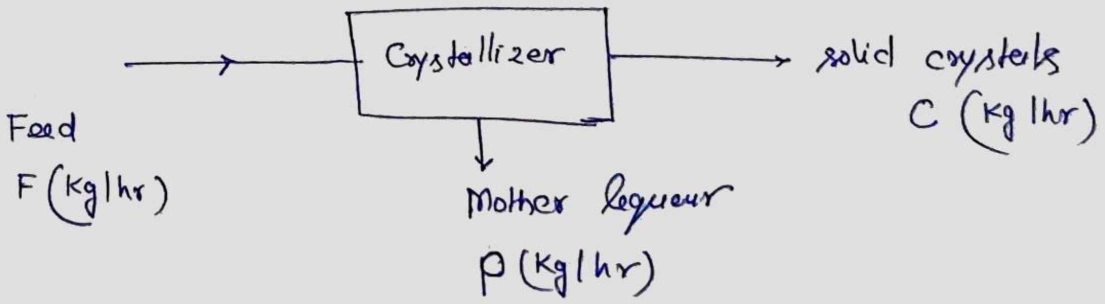
obsorption column :—



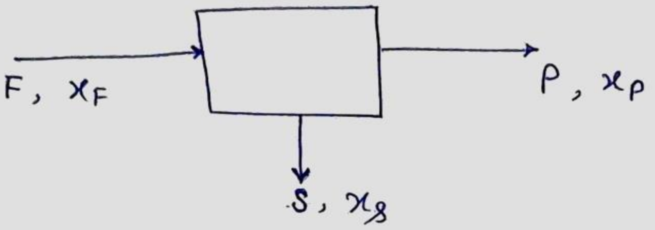
Example

abortion of NH_3 in water

Crystization :—



Material balance for unit operation —



1) overall material balance —

as system is steady state continuous process

rate of material in = rate of material out

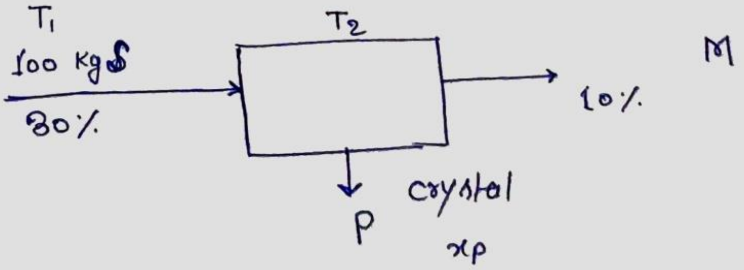
$$\boxed{F = P+S}$$

2) component balance —

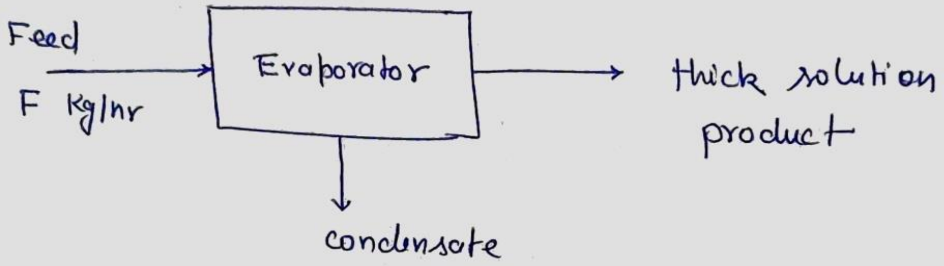
$$\boxed{F x_F = P x_p + S x_s}$$

Example - ①

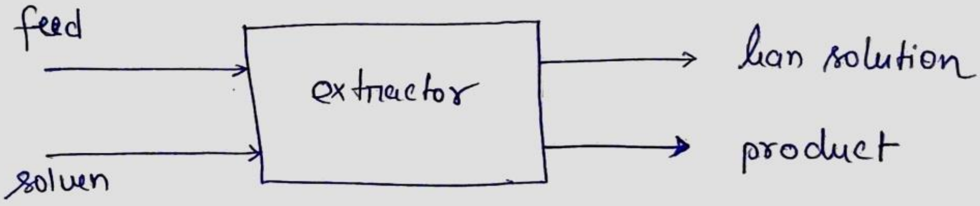
$Na_2SO_4 \cdot 10\,H_2O$ crystals are formed by cooling 100 Kg of 30% by weight aques solution of Na_2SO_4. the final concentration of the solute in the solution is 10%. the weight of crystals is —



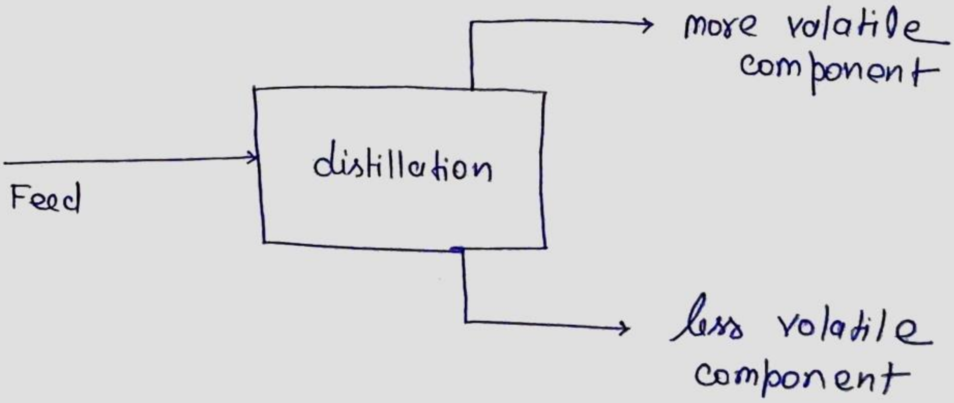
evaporation :-



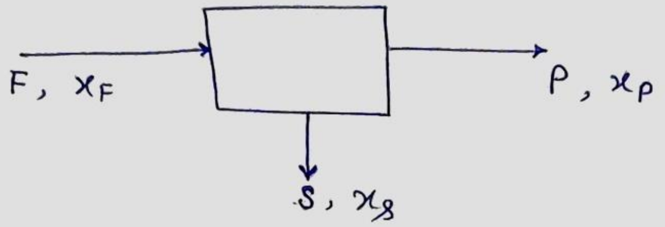
Liquid Extraction :-



Distillation :-



Material balance for unit operation —



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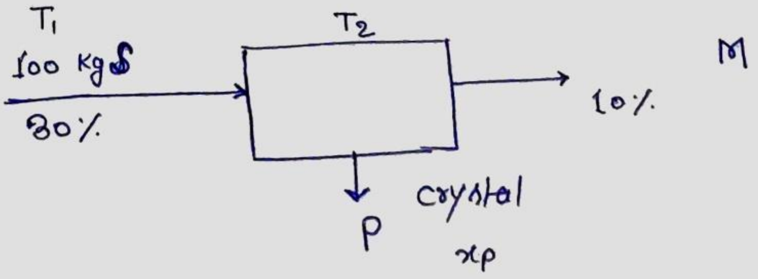


✓ overall matrial balance —

$$100 = P + M$$

✓ Na_2SO_4 balance —

$$100 \times \frac{30}{100} = P x_p + \frac{10}{100} M$$

x_p is mole fraction of Na_2SO_4 in crystal

1 mole crystal of $Na_2SO_4 \cdot 10 H_2O$ will contein,

1 mole Na_2SO_4 = 1 × 142 = 142 gm

10 mole H_2O = 10 × 18 = 180 gm

$$x_p = \frac{142}{142+180} = 0.44099$$

hence

$$30 = 0.441 P + 0.1 M$$

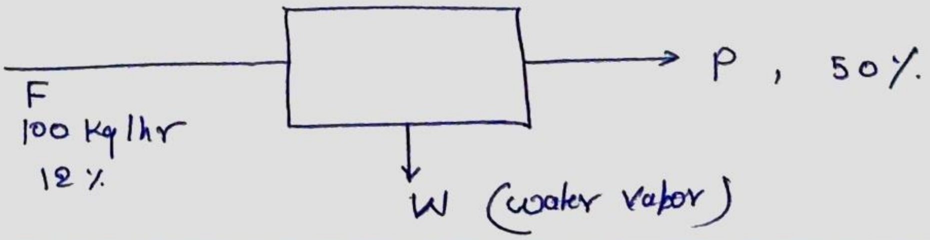
$$30 = 0.441 P + 0.1 (100 - P)$$

$$20 = 0.441 P - 0.1 P$$

$$P = 58.65 \text{ Kg/hr}$$

Example :—

Fresh orange juice conteins 12% (by weight) solids and rest water. 100 Kg/hr of juice is fed to evaporator to encrease solid content upto 50%. amount of water to be vaporized is — per hr basis



Tie Component :-

component in mixture which amount does not change during the operation is called tie component.

in above example : solid content of juice does not changes with the operation. hence it is tie component.

solution

overall material balance —

$$F = P + W \Rightarrow 100 = P + W \quad — ①$$

water balance — component

$$100 \times \frac{(100-12)}{100} = 0.5P + W \quad — ⑪$$

solving ① & ②

$P = 24$ Kg/hr

$W = 76$ Kg/hr

Ans = 76 Kg/hr

balance of tie component then solution of problem become easy

Method-② balance of tie component : solid content

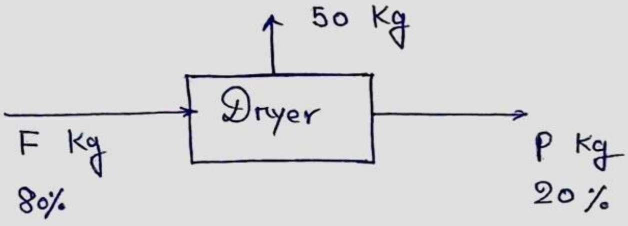
$$100 \times \frac{12}{100} = 0.5P \Rightarrow P = 24$$

$$P + W = 100 \Rightarrow W = 76 \text{ Kg/hr}$$

Lecture - 05 / Mass balance for unit operation - 02

Example :- Drying

A wet solid is dried upto 20% of moisture (by weight) from 80% of moisture (by weight). if evaporated water is 50 Kg then find the mass of wet solid.



Tie component = solid (dry)

component balance : dry solid

$$F(1-0.8) = P(1-0.2) \Rightarrow F = 4P$$

overall balance

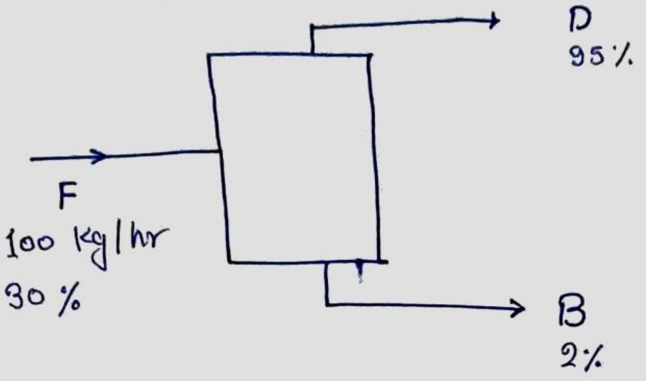
$$F = P + 50$$

solving $F = \frac{200}{3}$

---

* Distillation *

Methanol is separated from methanol + water solution using a distillation unit. Methanol obtained at Distillate is 95% pure & bottom product contains 2% of methanol. if feed is (100 Kg/hr, 30% methanol) then find Distillate flow rate



overall balance –

$F = D + B \Rightarrow D + B = 100$

methanol balance –

$0.3F = 0.95D + 0.02B \Rightarrow 0.95D + 0.02B = 30$

$D = 30.107$

$B = 69.892$

distillate flow rate = 30.107 kg/hr

---

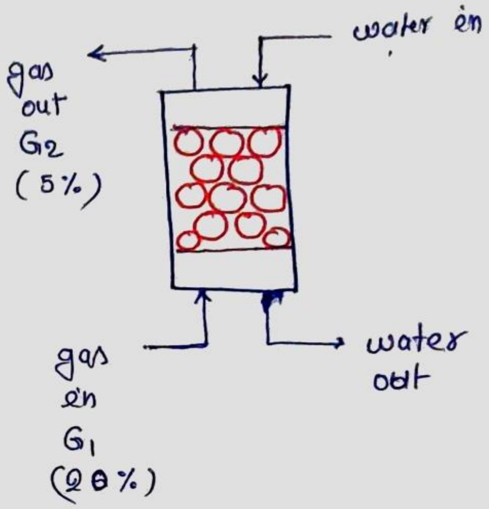
* Absorption *

Acetone is recovered from acetone-air mixture by using packed bed column and water used as solvent. Feed of gas mixture contains 20% of acetone by weight. gas mixture leaving the Column is 5% find % of acetone absorbed basis :-

inlet gas mixture 100 kg/hr

20 kg/hr acitone

80 kg/hr air



out let –

G_2 kg/hr

Tie component air –

air in = air out

$80 = G_2 \times 0.95 \Rightarrow G_2 = 84$ kg/hr

acitone at outlet $= 84 \times \frac{5}{100} = 4.21$ kg/hr

$$\% \text{ acitone absorbed} = \frac{\text{inlet} - \text{outlet}}{\text{inlet}} \times 100$$

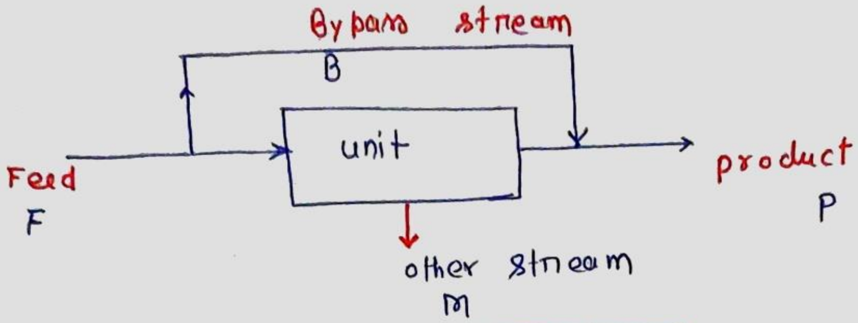
$$= \frac{20 - 4.21}{20} \times 100$$

$$= 78.94 \%$$

* By Pass *

to control and regularisation of product specification & concentration.

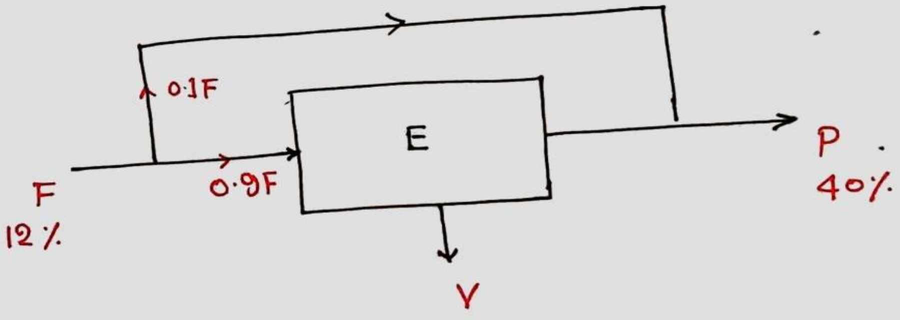
$$\text{By pass ratio} = \frac{\text{flow rate of by pass stream}}{\text{flow rate of fresh feed}}$$



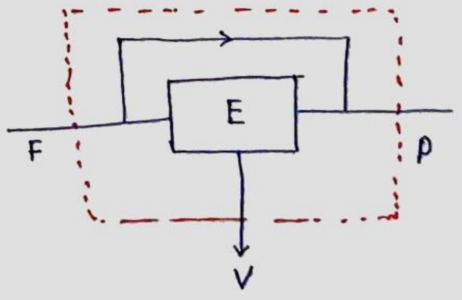
$$\boxed{\text{By pass ratio} = \frac{B}{F}}$$

Example :-

Fresh orange juice contains 12% (by weight) solids and the rest water. 90% of the fresh juice is sent to an evaporator to remove water and subsequently mixed with the remaining 10% of fresh juice. The resultant product contains 40% solids. the amount of water removed from 1 Kg fresh juice is.



take unit as per figure



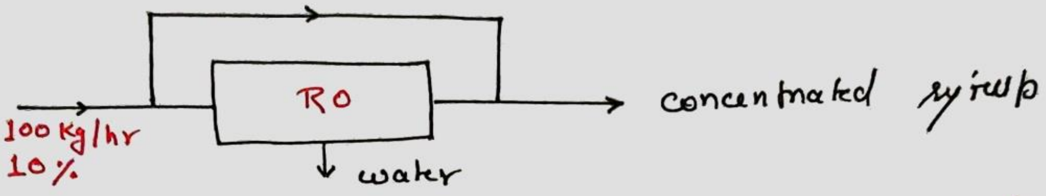
Tie component : solid content

$0.12F = 0.4P$

$P = 0.3 \text{ Kg}$

$F = P + V \qquad 1 = 0.3 + V \Rightarrow V = 0.7 \text{ Kg}$

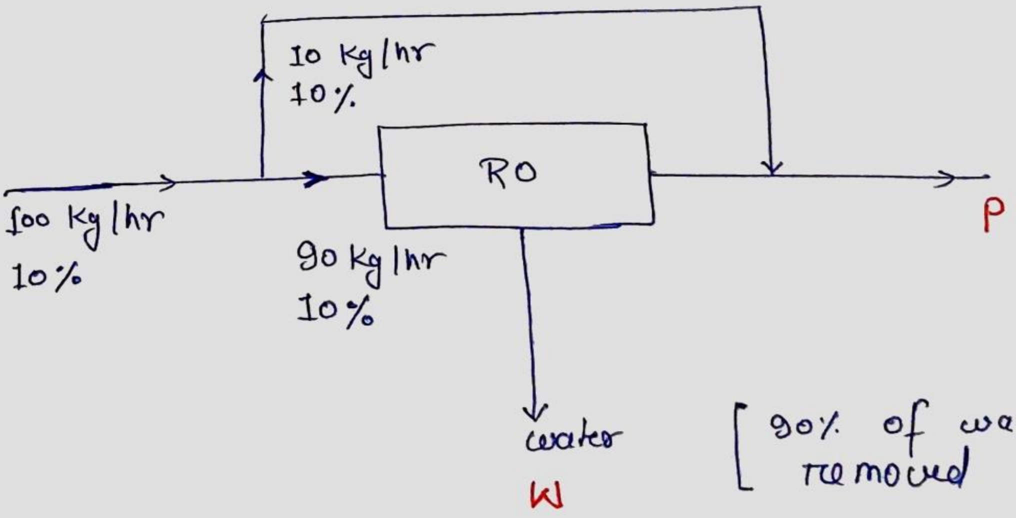
Example :-



Food processing endustry suger syrup to be concentrated by using reverse osmosis unit operation. RO unit remove 90% of water of it feed. 100 kg/hr Feed of 10% suger to be treated in 10% of it's in by pass scheme. find throughput & contentration of product (concentrated stream).

Solution :-

$$\text{Bypass ratio} = \frac{10}{100}$$



[90% of water will be removed]

Feed of RO - 90 kg/hr 10% suger

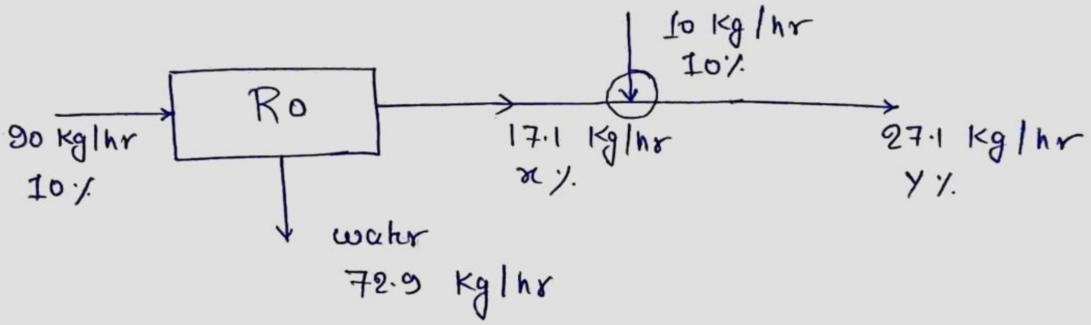
water $W = 90 \times (1-0.1) \times 0.9$

$W = 81 \times 0.9 \text{ kg/hr} = 72.9$

overall balance —

$100 = P + W \Rightarrow P = 100 - 72.9 = 27.1$ kg/hr

Now Ro unit —



component suger balance on RO —

$$90 \times 0.1 = 17.1 \times \frac{x}{100} \Rightarrow x = 52.63\ \%$$

component balance on junction where bypass and Ro output is meeting —

$$17.1 \times \frac{52.63}{100} + 10 \times 0.1 = 27.1 \times \frac{y}{100}$$

$$y = 36.9\ \%$$

hence out put suger concentration 36.9%.

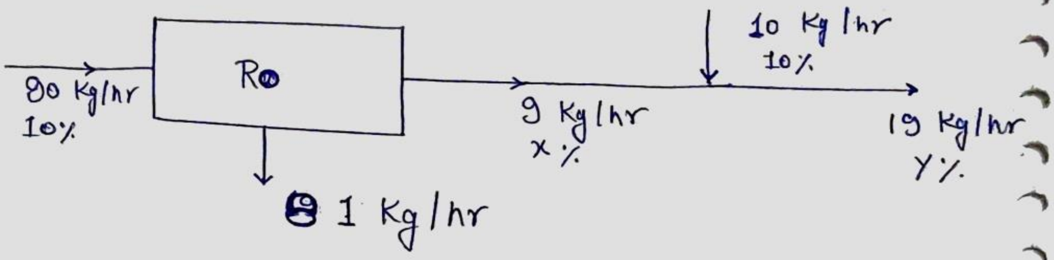
overall balance

$100 = P + \omega$

$P = 100 - 81$

$P = 19$ Kg/hr

now RO unit only



component balance — suger

$90 \times 0.1 = 9 \times \frac{x}{100}$ $x =$

90×0.9 water $= 81$ Kg/hr

$= 72.9$ Kg/hr

* Recycle *

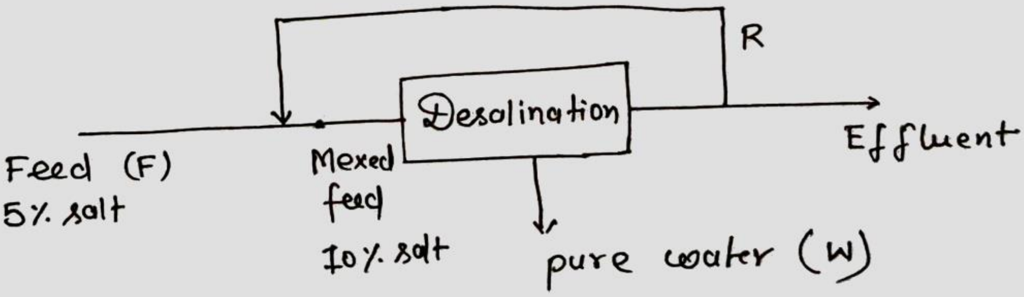
- to emprove conversion or degree of separation
- to emprove or control the product specification
- to conserve the energy.

Recycle Ratio —

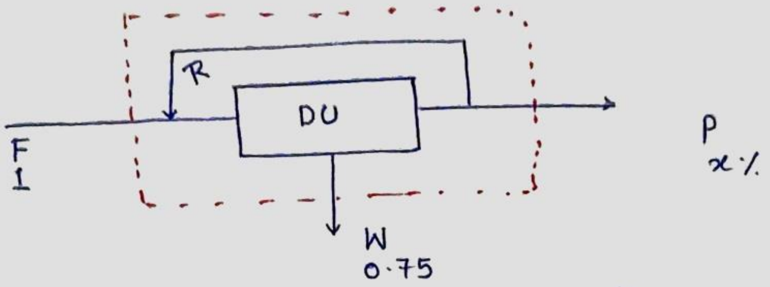
$$= \frac{\text{Amount of stream recycled}}{\text{Amount of fresh feed stream}}$$

Example :-

pure water (stream w) is to be obtained from a feed containing 5 (wt%) salt using a desalination unit as shown below —



If the overall recovery of pure water (through stream w) is 0.75 Kg/Kg feed, then the recycle ratio (R/F) is



$F = P + W$ — ovrall

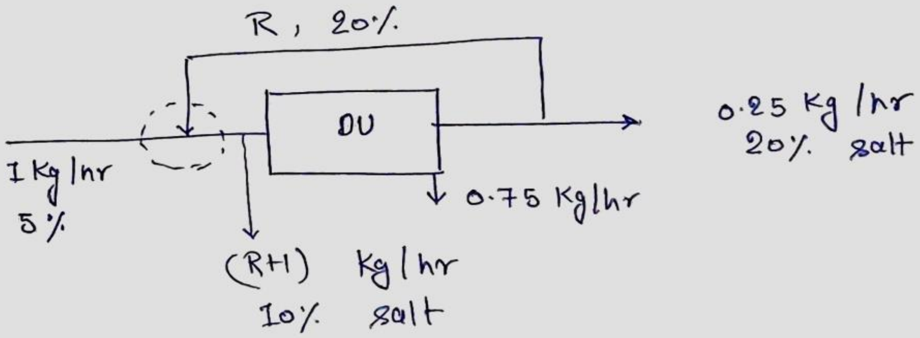
$0.05F = P \cdot \frac{x}{100}$ — component

basis ⇒ F = 1 Kg/hr

$W = 0.75$ Kg/hr ⟹ $P = 0.25$ Kg/hr

$x = 20$ %

balance at recycle junction :—



salt balance —

$1 \times 0.05 + R \times 0.2 = (R+1)\ 0.1$

~~0.05 = 0.3R x 0.1~~

$0.1R = 0.05$ $R = 0.5$ Kg/hr

$$\text{Recycle ratio} = \frac{R}{F} = \frac{0.5}{1} = 0.5$$

Ans

Lecture - 06 / Reaction Systems / unit process :-

Chemical Rxn -

$C + O_2 \longrightarrow CO_2$

$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$

$CaCO_3 + 2HCl \longrightarrow CaCl_2 + CO_2 + H_2O$

$MnO_2 + 4HCl \longrightarrow MnCl_2 + 2H_2O + Cl_2$

Stoichiometry -

Atomic balance for chemical Rxn

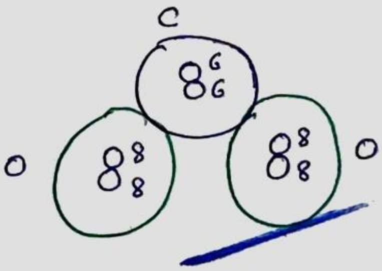
Atomic balance = conservation of mass

proof :- $C + O_2 \longrightarrow CO_2$

Lets take example of CO_2 molecule -

mass of one CO_2 molecule = 44 U = Mu

M = molecular mass of CO_2



mass of neutron

$= 1.66 \times 10^{-24} = 1\,U$

mass of protron

$= 1.66 \times 10^{-24} = 1U$

mass of carbon atom = 12 U

mass of O_2 molecule = 32 U

Σ mass of reactant = 12 U + 32 U

= 44 U

Σ mass of product = 44 U

$$\boxed{\Sigma \text{ mass of reactant} = \Sigma \text{ mass of product}}$$

Law of definite proportion :-

% mass of an element in a molecule is always definite or certain.

Example :- % of carbon in CO_2 molecule

$$= \frac{6U + 6U}{44U} \times 100$$

$$= 27.27\ \%$$

Example :-

find mass percent of Na in Na_2SO_4 -

$$= \frac{23 \times 2\ U}{(23 \times 2 + 32 + 16 \times 4)\ U} \times 100$$

$$= 32.39\ \%$$

Mole - Concept

Definite - 1 mol is amount of substance that contains as many as entities as there in C-12 of 12 gm.

→ mass of 1 atom of C-12 = $12 \times 1.66 \times 10^{-24}$ gm

$12 \times 1.66 \times 10^{-24}$ gm will contain 1 atom C-12

1 gm will contain $= \frac{1}{12 \times 1.66 \times 10^{-24}}$ C-12 atoms

12 gm will contain $= \frac{12}{12 \times 1.66 \times 10^{-24}}$ atoms

$= 6.022 \times 10^{+23}$ atoms

= Avegedro number

→ mass of 1 mol O_2 ?

$= 6.022 \times 10^{23} \times M \times 1.66 \times 10^{-24}$ gm

M: molecular mass of O_2

= M gm

= 32 gm

→ for any molecule

M gm — 1 mol

1 gm — $\frac{1}{M}$ mol

$$\boxed{w \text{ gm} - \frac{w}{M} \text{ mol}}$$

as mol is a number —

mol balance ⟶ atomic balance ⟶ conservation of mass

Example :-

find required HCl to react completly with 5 g MnO_2

$$MnO_2 + 4HCl \longrightarrow MnCl_2 + 2H_2O + Cl_2$$

moles of $MnO_2 = \frac{5}{87} = 0.057$ mol

4 mol HCl required for 1 mol MnO_2

0.057 mol MnO_2 requires $= 4 \times 0.057$ mol HCl

$= 4 \times 0.057 \times 36$ gm HCl

$= 8.27$ gm HCl

Average Molecular Mass :—

Que :- 100 gm sample of clorine. clorine has two isotopes in the sample Cl-35 & Cl-37 find average molecular mass.

Cl-35 — 75%
Cl-37 — 25%
} by mass present in sample

solution – M : average molecular mass of sample

Moles of Clorine = moles of Cl-35 + moles of Cl-37

$$\frac{100}{M} = \frac{75}{35} + \frac{25}{37}$$

$$M = 35.47$$

Excess & Limiting Reactant :—

If reactants given in stoichimetric proportion then after completion of rxn no any reactant will remain or all reactants will be consumed completly.

If reacts given are not in stoichiometric proportion then all reacts are not consumed entirly when rxn completes. The Reactant which exaust first is called Limiting Reactant and Reactant which remains is called excess reactant.

How to find Limiting & Excess Reactant :—

step ①. devide given mol of reactant initially with stoichiometric coefficient.

step ②. find out least division. Least division will be Limiting reactant.

Step ③. All other reactant will be excess reactant.

Example :—

CH_4 Reacts with O_2. find limiting and Excess reactant for the following cases —

1) 1 mol CH_4, 1 mol O_2
2) 1 mol CH_4, 2 mol O_2
3) 1 mol CH_4, 4 mol O_2

Case - I)

$$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$$

$$\begin{array}{cc} 1 & 1 \\ \frac{1}{1} & \frac{1}{2} \end{array}$$

] devision by stoichio-metric coefficient

least

Excess Limiting

Case - I)

$$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$$

$$\begin{array}{cc} 1 & 2 \\ \frac{1}{1} & \frac{2}{2} \end{array}$$

] devide by stoichiometric coefficient

equal

Heance Reactants are in stoichiometric proportion case - III)

$$\underbrace{\underset{\frac{1}{1}}{\underset{1}{CH_4}}}_{\text{least}} + \underset{\frac{4}{2}}{\underset{4}{2\,O_2}} \longrightarrow CO_2 + 2\,H_2O$$

Limiting Excess

% Excess :—

$$= \frac{\text{moles of reactent fed} - \text{Required mol of R}}{\text{Required mol of reactent}} \times 100$$

Example :—

0.75 M, HCl, 25 ml, to react compltly gm of $CaCO_3$ required if it is 20% in excess.

solution —

$$CaCO_3 + 2\,HCl \longrightarrow CaCl_2 + CO_2 + H_2O$$

moles of HCl present $= 0.75 \times 25 \times 10^{-3}$

$= 18.75 \times 10^{-3}$ moles

moles of $CaCO_3$ required to react completely $= \frac{1}{2} \times 18.75 \times 10^{-3}$

$$\% \text{ excess } CaCO_3 = \frac{\text{moles } \cancel{\text{Requ}} \text{ fed} - \text{Required}}{\text{Required}} \times 100 .$$

0.2 Required + Required = moles fed

moles fed = 1.2 Required

moles fed = $1.2 \times \frac{1}{2} \times 18.75 \times 10^{-3}$

gm $CaCO_3$ fed $= \frac{1.2}{2} \times 18.75 \times 10^{-3} \times 100$

$= 1.125$ gm

Example :—

for NH_3 formation Reaction, find limiting and excess Reactant for following Reactants —

	N_2	+	$3H_2$	$\longrightarrow$	$2NH_3$
1)	1 m		3 m		
2)	1 m		1 m		
3)	1 gm		1 gm		
4)	1 gm		3 gm		

Solution

	N_2	+	$3H_2$	
Case - I	$\frac{1}{1}$		$\frac{3}{3}$	] stoichimetric proportion
case - II	$\frac{1}{1}$		$\frac{1}{3}$	] H_2 limiting

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

case - III) $\frac{1}{28 \times 1}$ $\frac{1}{2\text{[illegible]} \times 3}$] N_2 limiting

gm must be converted into mol first

Case - IV) $\frac{1}{28}$ $\frac{3}{\text{[illegible]}\ 3}$] N_2 limiting

Lecture - 07 / Unit process / Material balance on Reactor

- Conversion
- Yield
- Selectivity
- Reactor Material balance

Conversion :-

$A \longrightarrow B$

$$\text{fractional Conversion} = \frac{\text{moles reacted}}{\text{moles fed to Reactor}}$$

$$\text{percentage conversion} = f \cdot c \times 100$$

fraction conversion of A

$$= \frac{\text{mol of A at inlet} - \text{mol of A out}}{\text{mol of A inlet}}$$

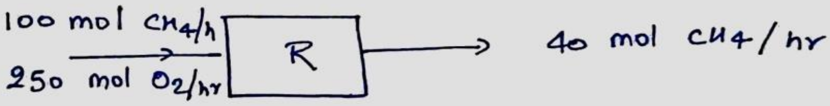
→ overall material balance on Reactor – (steady state)

$$\text{in} - \text{out} = 0$$

→ component balance on Reactor – (steady state)

$$(\text{in} + \text{generation}) - (\text{out} + \text{disappearance}) = 0$$

Example :–



$$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$$

1) find % conversion of CH_4
2) outlet flow Rate of product
3) find % conversion of O_2

Solution :–

$$\text{conversion of } CH_4 = \frac{\text{in} - \text{out}}{\text{in}} \times 100$$

$$= \frac{100 - 40}{100} \times 100$$

$$= 60 \text{ \%}$$

	CH_4 +	$2O_2$ ⟶	CO_2 +	$2H_2O$
inlet	100	250		
outlet	(100 – 60)	(250 - 2×60)	40	60×2

ⓐ out let –

$CH_4 = 40$

$O_2 = 130$

$CO_2 = 60$

$H_2O = 120$

---

total = 350 mol/hr

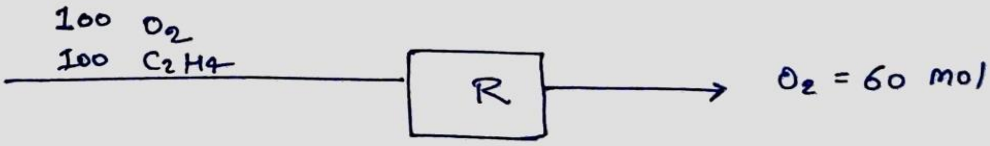
$$\% \text{ conversion of } O_2 = \frac{\text{in} - \text{out}}{\text{in}} \times 100$$

$$= \frac{250 - 130}{250} \times 100$$

$$= 48 \%$$

Example :–

$$2C_2H_4 + O_2 \longrightarrow 2C_2H_4O$$



find fractional conversion of limiting Reactant

	$2C_2H_4$ +	O_2 $\longrightarrow$	$2C_2H_4O$
inlet	100	100	
outlet	$(100 - 40 \times 2)$	$(100 - 40)$	2×40

Limiting Reactant = C_2H_4

$$\% \text{ conversion of } C_2H_4 = \frac{\text{in} - \text{out}}{\text{in}}$$

$$= \frac{100 - 20}{100}$$

$$= 0.8$$

Yield :-

Multiple Rxn —

$$A+B \begin{cases} \rightarrow C+D & \text{(desirable)} \\ \rightarrow E+F & \text{(undesirable)} \end{cases}$$

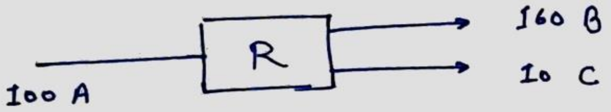
$$A+B \longrightarrow C+D \longrightarrow E+F$$

$$\text{Yield} = \frac{\text{moles of desired product formed}}{\text{moles of desired product formed if there is no side rxn and limiting Reactant consumed completly}}$$

Selectivity :-

$$\frac{\text{moles of desired product formed}}{\text{moles of undesired product formed}}$$

Example :-



find

1) conversion of A
11) % yield of desired product
111) Selectivity

Solution :-

A consumed to form 160 B = 80 mol

A consumed to form 10 C = 10 mol

total A consumed = 80 + 10 = 90 mol

$$\% \text{ conversion of } A = \frac{90}{100} \times 100 = 90$$

moles of desired product formed if there is no side Rxn and A completly consumed

= 200 mol

$$\% \text{ yield} = \frac{160}{200} \times 100 = 80\%$$

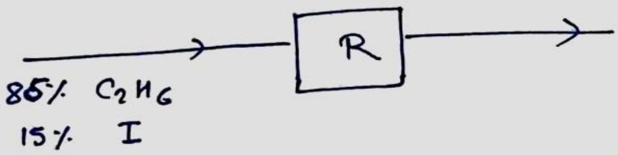
$$\text{Selectivity} = \frac{160}{10} = 16$$

Example :—

Dehydrogenation Rxn —

$C_2H_6 \longrightarrow C_2H_4 + H_2$ (Desired Rxn)

$C_2H_6 + H_2 \longrightarrow 2\,CH_4$



fractional conversion of ethylene = 0.501

yield = 0.471

find —

1) outlet compositions —

2) Selectivity C_2H_4 / CH_4

Solution :—

basis :— 100 mol/hr Reactant

$C_2H_6 = 85$ $\qquad$ I = 15

$$\text{conversion of } C_2H_6 = 0.501 = \frac{85 - \text{outlet}}{85}$$

outlet $C_2H_6 = 42.415$

Yield = 0.471

moles of desired product formed if there is no side Rxn = 100 × 0.85

$$\begin{array}{ccccc} C_2H_6 & \longrightarrow & C_2H_4 & + & H_2 \\ 100\times0.85 & & & & \\ 0 & & 100\times0.85 & & 100\times0.85 \end{array}$$

hence

$$0.471 = \frac{C_2H_4 \text{ formed}}{85}$$

C_2H_4 formed = 40 moles

hence H_2 formed = C_2H_4 formed = 40 moles

C_2H_6 consumed in desired Rxn = 40 moles

total C_2H_6 consumed = 42.585 moles

C_2H_6 consumed in side rxn = 42.585 − 40

= 2.585 moles

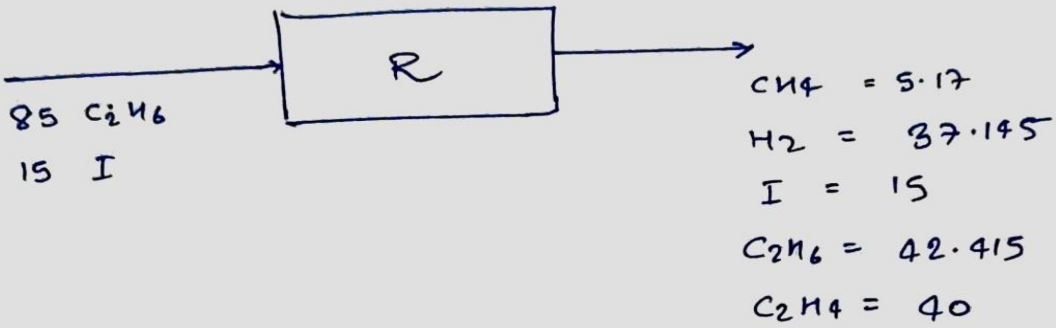
side Rxn —

$$\begin{array}{ccccc} C_2H_6 & + & H_2 & \longrightarrow & 2CH_4 \\ -2.585 & & -2.585 & & 2\times2.585 \end{array}$$

H_2 consumed = −2.585

hence H_2 at outlet = 40 − 2.585 = 37.415

CH_4 at outlet = 2 × 2.585 = 5.17


R
85 C_2H_6
15 I
CH_4 = 5.17
H_2 = 37.145
I = 15
C_2H_6 = 42.415
C_2H_4 = 40

Lecture - 08 / Unit Process / Combustion Reaction :-

Burning of Hydrocarbon -

$$C_xH_y + \left(x+\frac{y}{4}\right)O_2 \longrightarrow xCO_2 + \frac{y}{2}H_2O$$

Incomplete combution -

Example : CH_4

$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$ complete

$CH_4 + \frac{3}{2}O_2 \longrightarrow CO + 2H_2O$ Incomplete

$$\%\ \text{excess Air} = \frac{\text{Air Supplied} - \text{theoretical air demand}}{\text{theoretical air Demand}} \times 100$$

$$\%\ \text{excess } O_2 = \frac{O_2 \text{ supplied} - \text{theoretical } O_2 \text{ required}}{\text{theoretical } O_2 \text{ required}} \times 100$$

Composition of air — (79% N_2 , 21% O_2)

theoretical air Required is calculated by considering complete combution rxn in which CO_2 & H_2O is formed.

Example :—

the product combution of CH_4

CO_2 : 7 mol
CO : 2 mol
N_2 : 83 mol
O_2 & H_2O

find % excess air supplied —

Solution : –

$$(I) \quad CH_4 + 2O_2 \longrightarrow \underset{7}{CO_2} + 2H_2O$$

$$(II) \quad CH_4 + \frac{3}{2}O_2 \longrightarrow \underset{2}{CO} + 2H_2O$$

CH_4 is not at outlet ~~of~~ Combustor —

CH_4 consumed in 1st rxn = 7 mol

CH_4 consumed in 2nd rxn = 2 mol

hence total CH_4 supplied = 9 mol

O_2 required for complete combustion of CH_4 = 18 mol

$$O_2 \text{ supplied} = \frac{83}{0.79} \times 0.21 = 22.063$$

$$\% \text{ excess } O_2 = \frac{22.063 - 18}{22.063} \times 100$$

$$= 22.57\,\%$$

% excess air = 22.57 %

Ans:—
22.57%

Example –

I mol CH_4 undergoes combution with stoichiometric amount of air. Reaction is

$$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$$

find mol fraction of H_2O in flue gases if conversion of CH_4 is 80%.

Solution –

	CH_4 +	$2O_2$ $\longrightarrow$	CO_2 +	$2H_2O$
t= 0	1	2	0	0
80% conversion	$(1-0.8\times1)$	$(2-0.8\times2)$	0.8×1	0.8×2

basis : 1 mol CH_4 supplied –

O_2 supplied = 2 mol , as it is in stoichiometric proportion.

N_2 supplied $= \frac{2}{0.21} \times 0.79 = 7.52$

hence —
at outlet of combustor —

$CH_4 = 0.2$
$O_2 = 0.4$
$N_2 = 7.52$
$CO_2 = 0.8$
$H_2O = 1.6$

$$\%\ H_2O = \frac{1.6}{1.6+0.8+7.52+0.4+0.2} \times 100$$

$$= 15.21\ \%$$

Example - 03

15 g coak (80% C, by weight) is burnt with 145 gm air and produces 22 gm CO_2, 56 gm CO find conversion of limiting reactant.

Solution

CO_2 : $22/44 = 0.5$ mol CO_2

CO : $5.6/28 = 0.2$ mol CO

air supplied = $\frac{145}{29}$ =

O_2 supplied = $\frac{145}{29} \times 0.21 = 1.05$ mol

Carbon in coak = $\frac{15 \times 0.8}{12} = 1$ mol

$$C + O_2 \longrightarrow \underset{0.5}{CO_2}$$

$$C + \frac{1}{2}O_2 \longrightarrow \underset{0.2}{CO}$$

Limiting reactant = C

total C consumed = $0.5 + 0.2 = 0.7$

% conversion of C = ~~1 - 0.7~~ $\frac{0.7}{1} \times 100$

$= 70\%$

Ans

Example - 04

Combustion of CH_4.

75 mol CO_2 formed, 25 mol CO formed.

Conversion of CH_4 is 70%.

60% of supplied Oxygen consumed

find % excess air used —

$$\underset{}{CH_4} + \underset{72\times 2}{2O_2} \longrightarrow \underset{75}{CO_2} + 2H_2O$$

$$CH_4 + \underset{\frac{3}{2}\times 25}{\frac{3}{2}O_2} \longrightarrow \underset{25}{CO} + 2H_2O$$

CH_4 consumed $= 75+25 = 100$ mol

CH_4 supplied $= \dfrac{100}{0.7}$ (as conversion of CH_4 is 70%)

$= 142.857$ mol

O_2 consumed $= 75\times 2 + \frac{3}{2}\times 25$

$= 187.5$

O_2 supplied $= \dfrac{187.5}{0.6} = 312.5$ (60% O_2 consumed)

theoretical O_2 required $=$ CH_4 supplied $\times 2$

$= 142.857 \times 2$

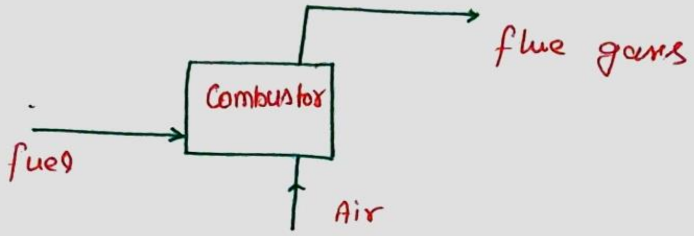
$= 285.71$

% excess O_2 = $\dfrac{312.5 - 285.71}{285.71} \times 100$

= 9.37 %

<u>Ans</u>

Lecture - 09 / Unit Process / Combustion / Orsat Analysis



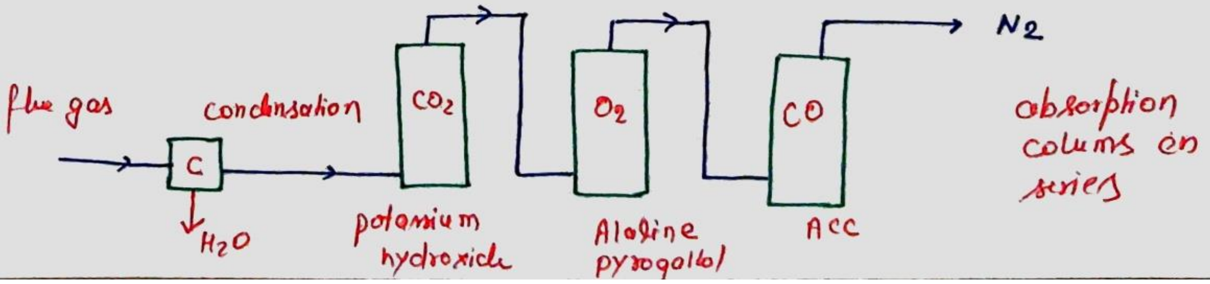
flue gas may contain —

- CO_2
- CO
- H_2O
- O_2
- N_2
- Unreacted reactants

as combution rxn is very fast, unreacted component in flue gases will be negligible —

Orsat Analysis :—

Orsat analysis is finding composition of components present in flue gases. Orsat Analyser is used for this purpose — (Dry basis composition)



Steps -

1) flue gases will be passed from condenser where H_2O vapor will be condensed out.

2) Remain gas mixure will be passed through series of absorption column. CO_2 is absorbed in potassium hydroxide column.

3) Remain gas contain (O_2, CO, N_2) will be passed through Alkaline pyrogallol column, where O_2 will be absorbed.

4) Last column is Ammonical cuprus cloride, where CO is absorbed. at outlet only N_2 will be present.

5) absrobed amount of (CO_2, O_2, CO) will be calculated. condensed H_2O will also be calculated

6) % composition of each component can be calculated (% CO_2, % O_2, % CO, % N_2). (H_2O composition not included in orsat)

Ques) A hydrocabon is burnt with excess air. orsat analysis gives.

% CO_2 = 10.81 %
% O_2 = 3.78 %
% N_2 = 85.40 %

find % excess air
C : H ratio of hydrocarbon

solution :- basis : 100 mol flue gas -

Air supplied = $\frac{85.40}{0.79}$ = 108 m

O_2 supplied = 108 × 0.21 = 22.70 m

O_2 consumed = 22.70 − 3.78 = 18.92 m

$$C_xH_y + \left(x+\frac{y}{4}\right)O_2 \longrightarrow x\,CO_2 + \frac{y}{2}H_2O$$

Required O_2 = O_2 consumed = 18.92 (as all C_xH_y ~~consed e~~ consumed in rxn)

% excess O_2 = $\frac{22.70 - 18.92}{18.92}$ = 19.97 %

CO_2 formed = 10.81 mol

$$\underset{1\text{ mol}}{C_xH_y} + \left(x+\frac{y}{4}\right)O_2 \longrightarrow x\,CO_2 + \frac{y}{2}H_2O$$

Consumed oxygen = $x + \frac{y}{4}$ = 18.92

CO_2 formed = 10.81 = x

y = 32.44

$\frac{x}{y} = \frac{10.81}{32.44} = \frac{1}{3}$

Que. CH_4 burnt in 30% excess air
90% of CH_4 produces CO_2, remaining CO
find composition in mol % of flue gases &
compare with composition obtain by orsat analysis —

Solution

basis: 100 mol CH_4

$$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$$
90

$$CH_4 + \frac{3}{2}O_2 \longrightarrow CO + 2H_2O$$
10

90 mol will be consumed in 1st rxn and 10 mol will be consumed in 2nd rxn.

$$\left.\begin{array}{l} CO_2 \text{ formed} = 90 \\ CO \text{ formed} = 10 \end{array}\right\} \text{at the outlet}$$

O_2 consumed $= 2 \times 90 + 10 \times \frac{3}{2} = 195$

theoretical O_2 required for CH_4 $= 2 \times 100 = 200$

supplied O_2 (30 excess) $= 1.3 \times 200 = 260$

O_2 at the outlet of reactor $= 260 - 195 = 65$

supplied N_2 $= \frac{260}{0.21} \times 0.79 = 978.09$

hence @ the outlet of combustor —

N_2 = 978.09
O_2 = 65
CO_2 = 90
CO = 10

Calcination :-

Conversion of carbonate, nitrate or sulphates into oxide by using heat. usually heat is produced by burning coal in presence of air.

$$CaCO_3 \longrightarrow CaO + CO_2$$
$$Cs(NO_3)_2 \longrightarrow CsO + NO_x$$

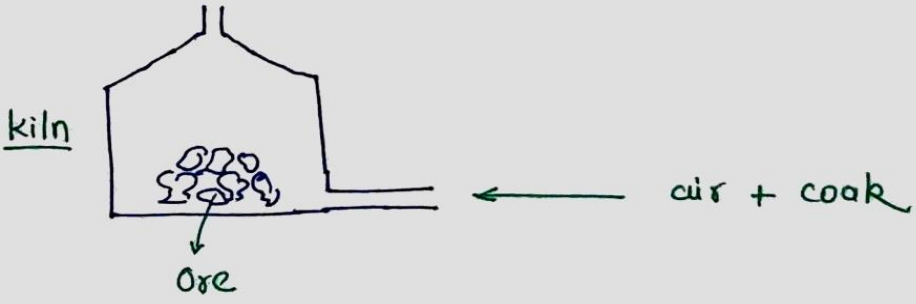


Fig : Calcination process

Example :-

Limestone — 84.5% $CaCO_3$, 11.5% $MgCO_3$, Rest Inert
burnt with coke (76% C, 21% ash, 3% moisture
Calcination of $CaCO_3$ ⇒ 95%.
$MgCO_3$ ⇒ 90%.

hence @ the outlet of combustor —

N_2 = 978.09
O_2 = 65
CO_2 = 90
CO = 10

Calcination :-

Conversion of carbonate, nitrate or sulphates into oxide by using heat. usually heat is produced by burning coal in presence of air.

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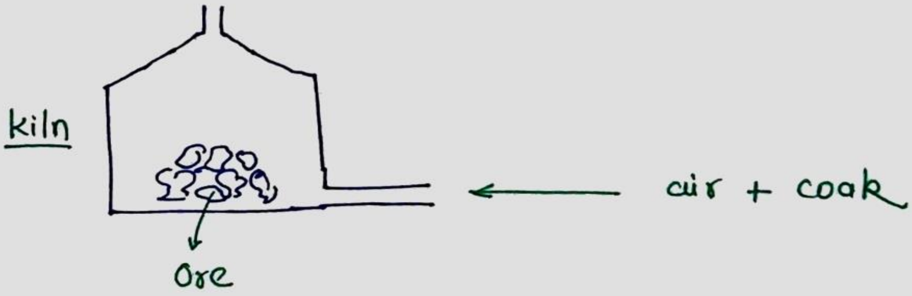


Fig : Calcination process

Example :-

Limestone – 84.5% $CaCO_3$, 11.5% $MgCO_3$, Rest Inert burnt with coke (76% C, 21% ash, 3% moisture

Calcination of $CaCO_3 \Rightarrow$ 95%.
$MgCO_3 \Rightarrow$ 90%.

Carbon in coak in completly burnt. the kiln is fed with 1 kg coak per kg of 5 kg limestone. Calculate weight % CaO in the solid leaving from kiln.

Solution

basis :- 1 kg limestone in fed

$$\left.\begin{array}{lll} CaCO_3 & = & 0.845\ kg \\ MgCO_3 & = & 0.115\ kg \\ I & = & 0.04\ kg \end{array}\right\}$$

0.2 kg coak (as 1/5)

ash = 0.21 × 0.2 = 0.042

$$CaCO_3 \longrightarrow CaO + CO_2$$

$$MgCO_3 \longrightarrow MgO + CO_2$$

Remain solid mixture of calcination will contein

$$\left\{\begin{array}{l} CaCO_3 \\ MgCO_3 \\ Inert \\ CaO \\ MgO \\ Ash \end{array}\right.$$

C will be complete conveted into CO_2 gas

90% conversion $MgCO_3$ / 95 % conversion of $CaCO_3$

$MgCO_3$ in solid mixture = $(1-0.90) \times 0.115$

= ~~0.0423~~ 0.0115

$CaCO_3$ in solid mixture = $(1-0.95) \times 0.845$

= 0.0423

Now we will calculate cao & MgO

molecular weight
$CaCO_3$ = 100
$MgCO_3$ = 84.3
CaO = 56
MgO = 40.3

$$CaCO_3 \longrightarrow CaO + CO_2$$

$\frac{0.845}{100}$ mol

$$CaO \text{ formed} = 0.95 \times \left(\frac{0.845}{100}\right) \times 56 \text{ Kg}$$

$$= 0.4495 \text{ Kg}$$

similarly MgO formed

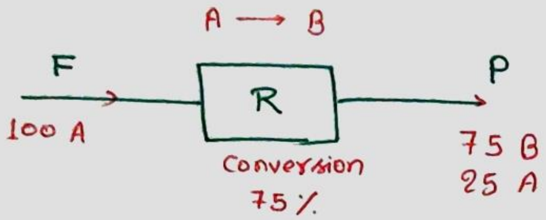
$$= 0.90 \times \left(\frac{0.115}{84.3}\right) \times 40.3$$

$$= 0.0495 \text{ Kg}$$

hence solid mixture will contain —

$CaCO_3$ = 0.0423 Kg
$MgCO_3$ = 0.0115 Kg
CaO = 0.4495 Kg
MgO = 0.0495 Kg
Inert = 0.04 Kg
Ash = 0.042 Kg

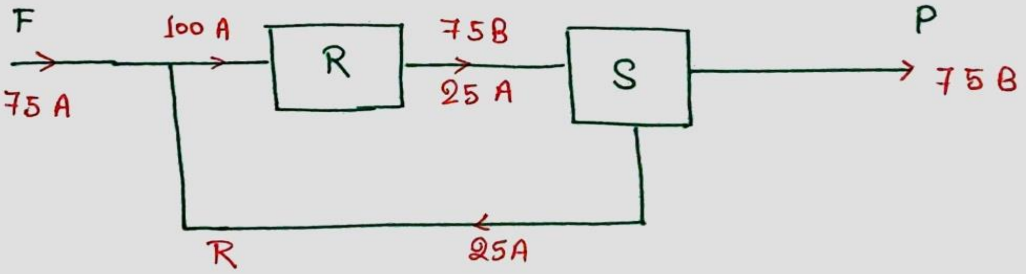
Lecture - 10 / Unit Process / Recycle Reactor



Conversion of Reactor is 75%.

* hence 100 mol of A will produce 75 mol B 25 mol A will remain unreacted, hence it is waste.

→ Now we will incorporate separator unit and unreacted material will be recycled

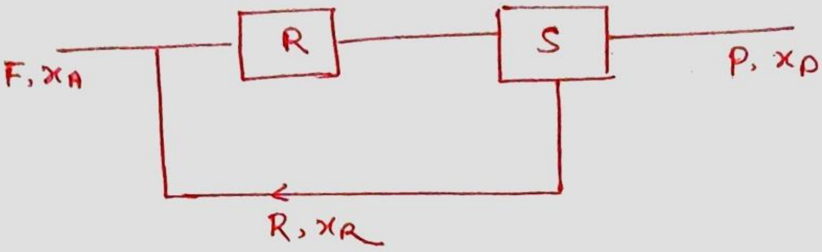


* in this case 75 A mol will produce 75 mol of B, hence no reactant will be lost.

Definition :—

1) Recycle Ratio = $\dfrac{\text{flow rate of Recycle stream}}{\text{flow rate of feed stream}}$

2) Overall Conversion —



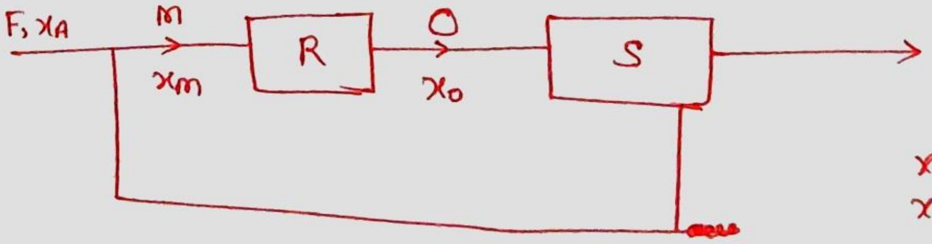
x_F, x_P, x_R } mol fractions

$$= \frac{F x_A - P x_P}{F x_A} \times 100$$

$$= \frac{\text{Reactan A in feed} - \text{Reactant in final product}}{\text{Reactant in feed}} \times 100$$

* if separator unit is 100% efficient, then Reactant in final product will be zero, hence Over all conversion will be 100%.

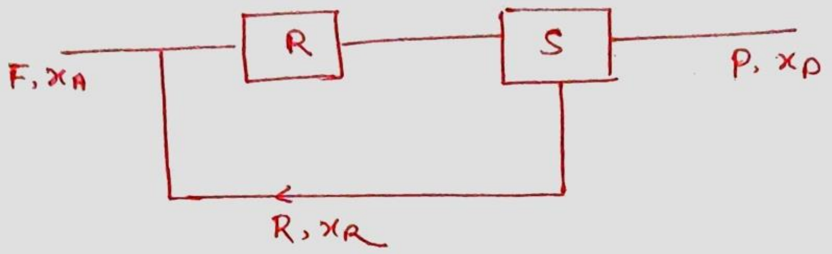
3) Single pass conversion : —



x_m, x_o } mol fraction

$$= \frac{M x_m - O x_o}{M x_m} \times 100$$

2) Overall Conversion —



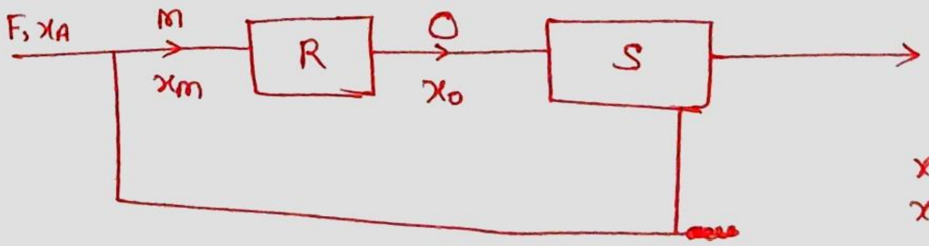
x_F
x_p
x_R
} mol fractions

$$= \frac{F x_A - P x_p}{F x_A} \times 100$$

$$= \frac{\text{Reactan A in feed} - \text{Reactant in final product}}{\text{Reactant in feed}} \times 100$$

* if separator unit is 100% efficient, then Reactant in final product will be zero, hence Over all conversion will be 100%.

3) Single pass conversion : —



x_m
x_o
} mol fraction

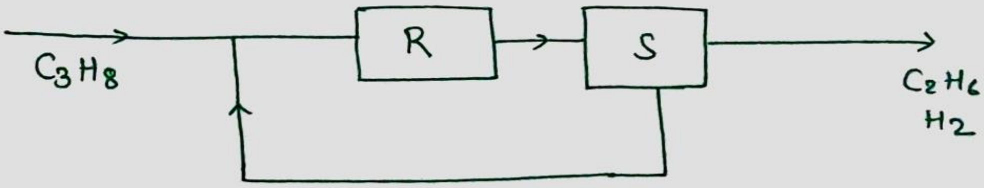
$$= \frac{M x_m - O x_o}{M x_m} \times 100$$

$$= \frac{\text{Reactant entering to Reactor} - \text{Reactant just after Reactor}}{\text{Reactant entering to Reactor}} \times 100$$

* Overall conversion is always greater than the single / one pass conversion

---

Example - 01)



$C_3H_8 \longrightarrow C_3H_6 + H_2$

→ Single pass conversion of reactor 40%

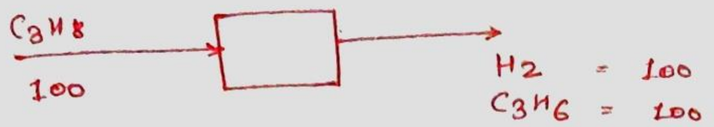
find

1) Recycle Ratio
2) Overall conversion : separator completly separates

Solution -

basis - 100 mol C_3H_8 at feed

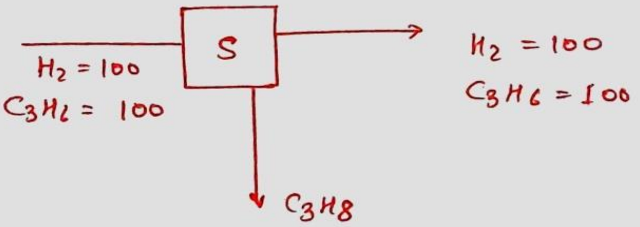
material balance on complete unit



→ there is no C_3H_8 at the outlet, hence all will be converted in to H_2 & C_3H_6

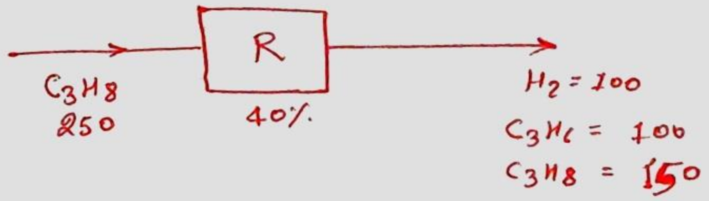
C_3H_8	$\longrightarrow$	H_2	+	C_3H_6
100				
0		100		100

→ now take separator unit –



at inlet of sepactor 100 mol H_2 , 100 mol

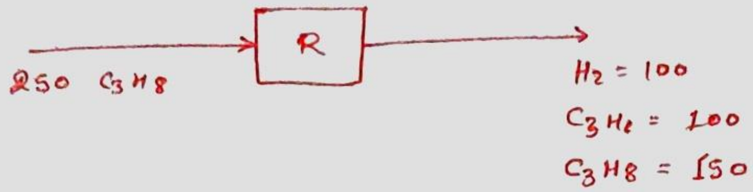
→ now we will take reactor unit –



C_3H_8 at inlet = x

$0.40\,x = 100 \implies x = 250$

C_3H_8 at the outlet = 150 = 250 − 100



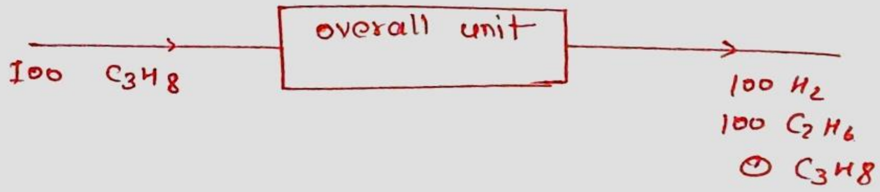
separator unit outlet C_3H_8 = C_3H_8 at outlet of Reactor

= 150 mol

Recycle stream flow = 150 mol

Recycle ratio = $\frac{R}{F} = \frac{150}{100} = 1.5$

Overall Conversion =

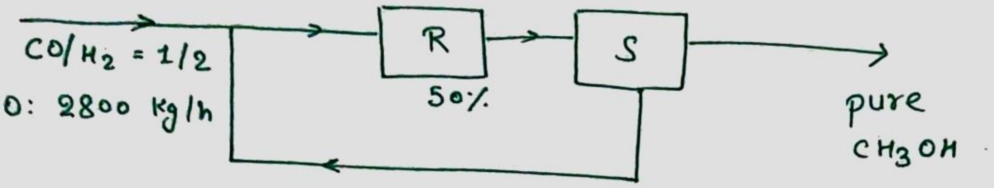


% conversion = $\frac{100 - 0}{100} \times 100$

= 100

Example –

$$CO + 2H_2 \longrightarrow CH_3OH$$



find

1) Recycle Ratio = R/F
2) Production rate of CH_3OH

molar ratio of CO & H_2 is 1/2 . single pass conversion of reactor is 30% .

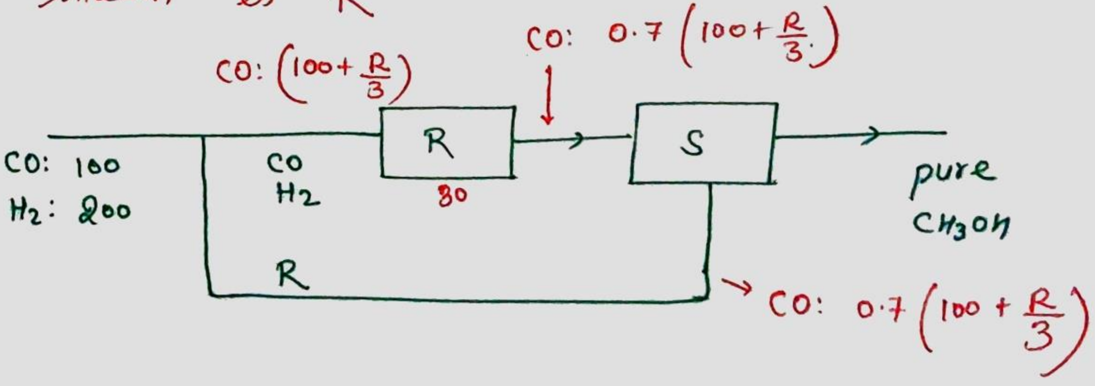
Solution

CO: $\frac{2800}{28}$ K mol / hr = 100 K mol / hr

H_2: 200 K mol / hr

CO and H_2 are in stoichiometric proportion hence all stream CO/H_2 ratio will be 1/2

→ Let assume that the flow rate of recycle stream is R



→ CO at the inlet of Reactor = $\left(100 + \frac{R}{3}\right)$

→ CO at the outlet of Reactor = $0.7\left(100 + \frac{R}{3}\right)$

→ CO at the Recycle Stream = $0.7\left(100 + \frac{R}{3}\right)$

hence

$$\frac{R}{3} = 0.7\left(100 + \frac{R}{3}\right)$$

$$R = 700$$

→ Recycle Ratio —

$$= \frac{700}{300}$$

$$= 7/3$$

→ single pass conversion = 30%

CH_3OH at outlet of Reactor = $0.3\left(100 + \frac{R}{3}\right)$

= 100 kmol/hr

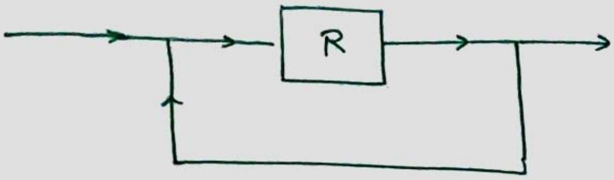
= 3200 Kg/hr

→ CH_3OH by overall balance —

CO	+	$2H_2$	→	CH_3OH
100		200		
0		0		100

hence production rate = 3200 Kg/hr

Example :-



→ isomerisation rxn $A \rightarrow B$

→ single pass conversion is 70%

→ Feed is pure A and R/F = 1.2

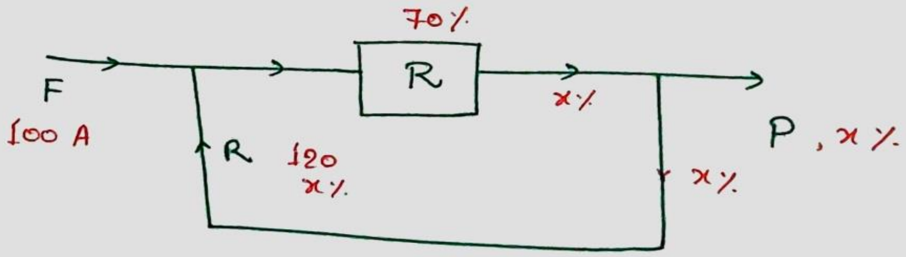
→ Overall conversion = ?

Solution

100 mol A @ Feed

$$\frac{R}{F} = 1.2 = \frac{R}{100} \Rightarrow R = 120$$

now percentage of A in outlet stream = x%

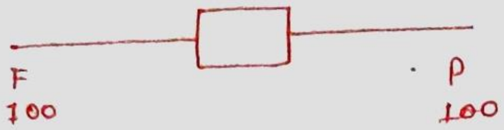


→ A at the inlet of reactor $= 100 + 120 \times \frac{x}{100}$

$= 100 + 1.2x$

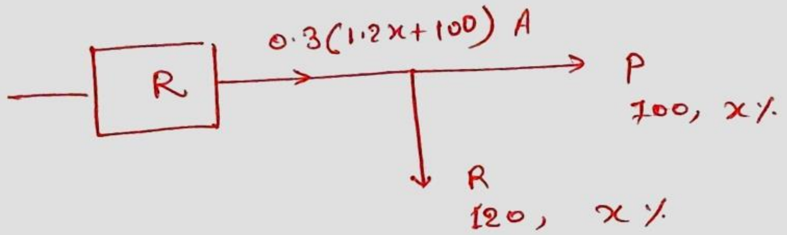
→ A at the outlet of reactor $= 0.3(100 + 1.2x)$

→ balance on overall unit -



$\text{in} = \text{out} = 100$

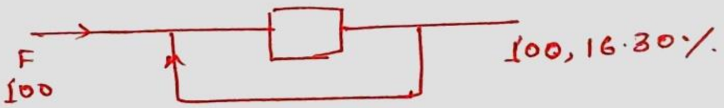
→ balance on the junction of outlet of reactor —



$$0.3(1.2x + 100) = 100 \times \frac{x}{100} + 120 \times \frac{x}{100}$$

$x = 16.30$

→ overall conversion —

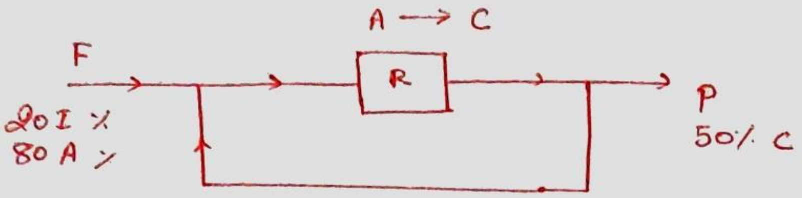


$$= \frac{100 - 100 \times \frac{16.30}{100}}{100} \times 100$$

$= 83.7\ \%$

→ overall conversion 83.7 % > single pass conversion 70%

When Feed contains Inert —



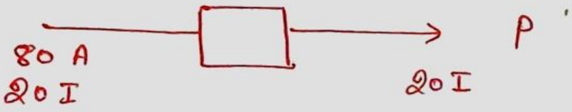
→ Feed contains 20% . R/F = 0.4

Product stream contains 50% C

find single pass conversion / overall conversion

Solution – 100 mol @ feed : basis

overall balance — inlet inert = outlet inert = 20



$P = 100$

C at outlet = 0.5 P = 50

unreacted A at outlet of reactor = 100 − 50 − 20

= 30

hence product stream contains 30% A

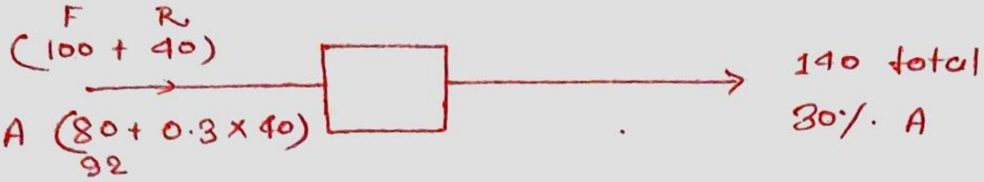
→ % of A in recycle stream = 30

→ R/F = 0.4 ⇒ R = 40

→ A at the inlet of reactor —

= 80 + 0.3 × 40 = 92

bolance of Reactor —



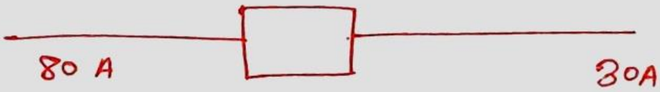
total mols in = total mols out = 140

A at outlet of reactor = 140 × 0.30 = 42

→ Single pass conversion $= \frac{92 - 42}{92} \times 100$

$= 54.34\ \%$

→ Overall conversion $= \frac{80 - 30}{80} \times 100 = 62.5\ \%$



Lecture-11/Unit Process/ Purge

$A \longrightarrow B$

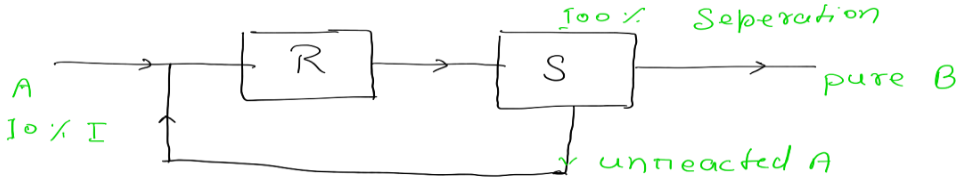
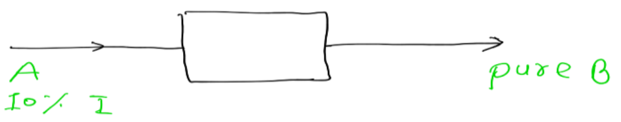


Fig: Feed with enert in Recycle reactor

What will happen to the reaction mixture Inert is entering in the system with fed but at the out let only pure B. hence we will apply Inert balance on complete system



$$\text{in} - \cancelto{0}{\text{out}} = \text{accumulation}$$

$$\text{in} = \text{accumulation}$$

hence with time Inert will start pile up in the reaction system. hence Reactant A will be diluted with inert. second problem will be pressurisation of Reactor in case of gas reaction & overflow of reactor in case of liquid rxn due to accumuation of inert onto the system.

Problem due to Inert in feed —

(I) Dilution of rxn mixture

(II) pressurization / over flow

Why we feed Inert into feed —

(I) to create protective gas environment.

(II) Raw material separation constrain

(I) Some times we need to add enert gases like Ar, Ne into the flamable gases to prevent it from auto egnition. hence we add enert intensionly into the feed for safe operation

(II) Many time it is not possible to separate feed reactant 100% hence during separation of raw material some enert remains in feed.

Purge Method is used to solve the problem caused by enert.

Example :—

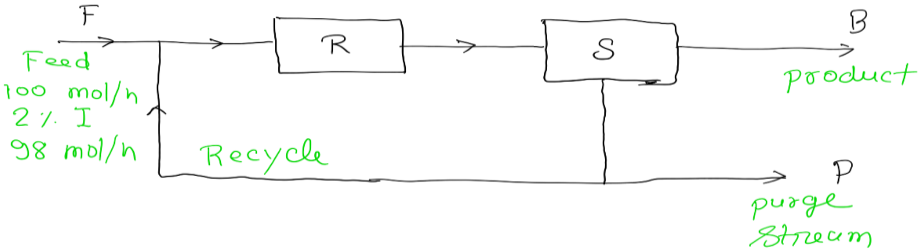
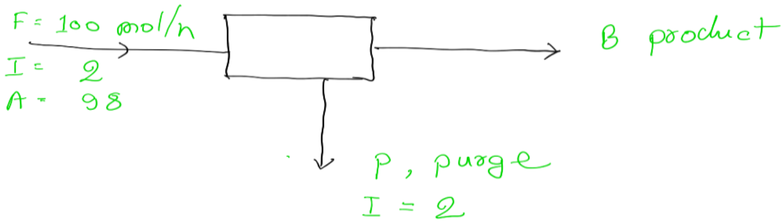


Fig : Recycle & Separator unit with purge

Inert balance on overall unit —



$$in - out = 0$$ (steady state Reactor)

$$2 - I_{out} = 0$$

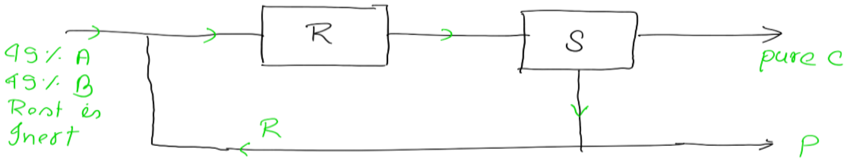
$$I_{out} = 2$$

hence all the enert present in the feed will come out of system through purge stream. no accumulation of enert will happen in the system hence dilution, overflow or pressurisation can be solved by purging some percentage of recycle stream.

Disadvantage of purge –

Some fraction of reactant will be lost in purge stream.

Example :–



$$A + B \longrightarrow C$$

given –

- maximum allowable concentration in Recycle stream is 10%

find –

- minimum P/F ratio ?
- loss of reactant per mol (A+B) fed

Solution –

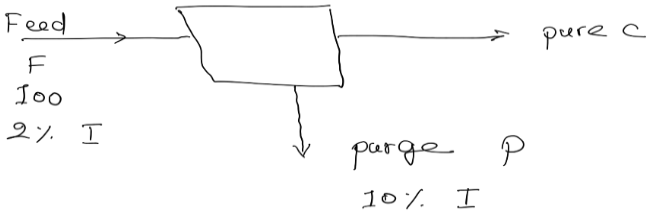
basis : 100 mol @ feed

A = 49 mol

B = 49 mol

I = 2 mol

Inert balance on overall unit –



in – out = 0

$$100 \times \frac{2}{100} - P \times \frac{10}{100} = 0$$

$$P = 20$$

$$P/F \text{ ratio} = \frac{20}{100} = 0.20$$

Ans

A+B in purge stream – 90%

$= 0.90\ P$

$= 18$ mol (will be lost)

A+B in feed = $49 + 49 = 98$

A+B lost in purge stream / (A+B) feed

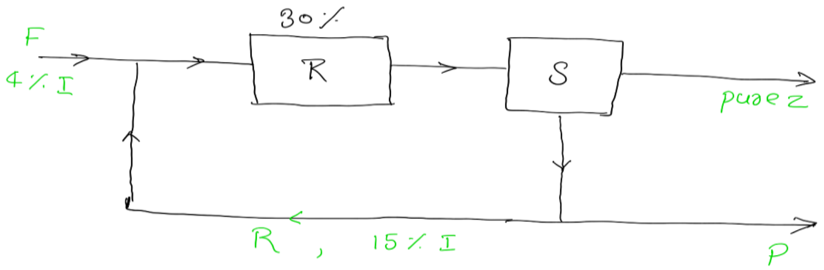
$= \frac{18}{98}$ Ans

Example :-

$2x + y \longrightarrow z$

x & y in feed is in stoichiometric proportion. separator separtes pure z completly. Inert in feed is 4 % Single pass conversion is 30 %. find

- Reactant loss per unit molar flow of x & y
- Recycle ratio
- Production rate of z



given that the inert in recycle stream is 15 %.

Solution :-

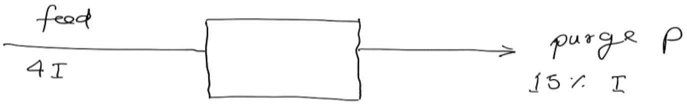
basis : 100 mol feed

I = 4 mol

x = 64 mol

y = 32 mol

overall unit, Inert balance —



% of inert in purge stream and recycle stream will be equal = 15%

$$in - out = 0$$

$$4 - 0.15\ P = 0$$

$$P = 26.66$$

(x + y) in purge stream = 85%

= 0.85×26.66

= 22.66

Inert in purge stream = 0.15 × 26.66

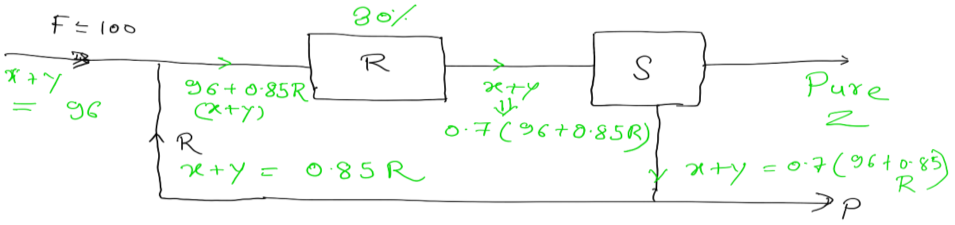
= 4

Hence Reactant loss per unit molar inlet flow of x & y

$$= \frac{22.66}{9.6}$$

$$= 0.236$$ Ans

Now recycle ratio —



x+y in feed = 96

x+y in recycle stream = 0.85 R

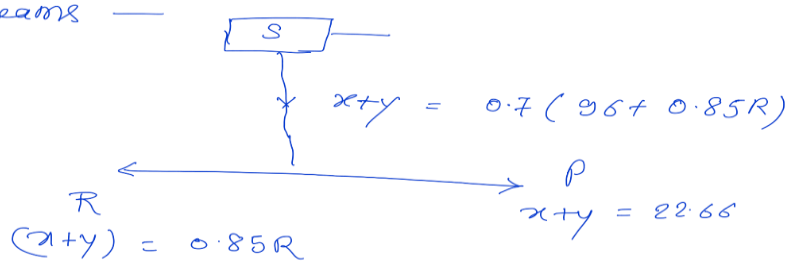
x+y at inlet of reactor = 96 + 0.85 R

x+y at outlet of reactor = 0.7 (96 + 0.85R)

x+y out from separator

= 0.7 (96 + 0.85 R)

x+y balance on Recycle and purge streams —



$$0.7 (96 + 0.85 R) = 0.85 R + 22.66$$

$$R = 174.66$$

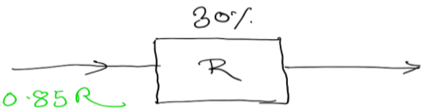
$$R/F = \frac{174.66}{100} = 1.74$$ Ans

Now production rate of Z →

$$2x + y \longrightarrow z$$

y consumed in reactor = production of z

balance on Reactor —



$$Y = \frac{96 + 0.85R}{3}$$

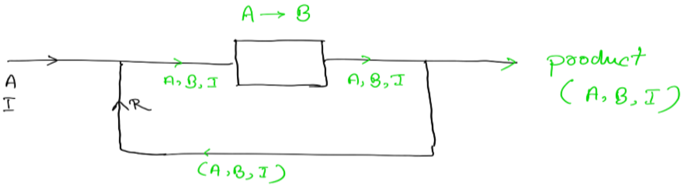
$$Z = \frac{0.3 (96 + 0.85R)}{3}$$

production of Z =

$$= \frac{0.8\,(96 + 0.85 \times 174.66)}{3}$$

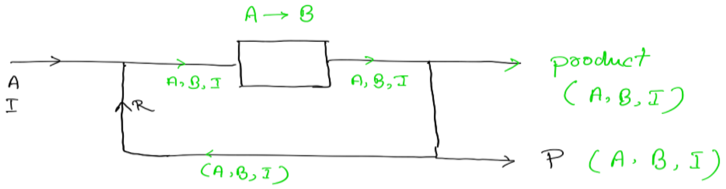
$\simeq$ 24.44 mol/hr Ans

purge without Separator unit :—



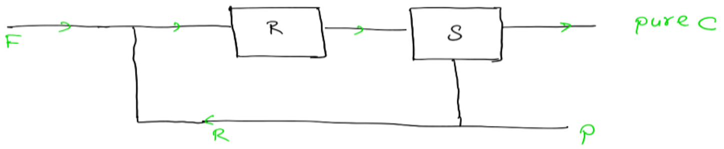
All the enert entring to the reactor will come out in product stream. Rxn mixture will be diluted to certain level upto the steady state reached.

If we purge in above system then dilution of reactor can be reduced upto some extent.



Requirment of purging for secondry product —

A ⟶ B + C



In above rxn, A will be converted into B & C As C is desired product and B is undesired, pure C is separated from separator unit.

Product B will start accumulating into the system hence it must be removed out of system to prevent accumulation. for this purpose some fraction of Recycle stream will be purge and rate of outlet of B at the purge will be equal to the rate of formation of B at the steady state.

Lecture - 12

Unsteady State Process

→ general material balance —

(in + generation) − (out + disappearance) = accumulation

accumulation term will appear in unsteady state process.

→ overall and component balance for unit operation —

in − out = accumulation

→ overall material balance for unit process

in − out = accumulation

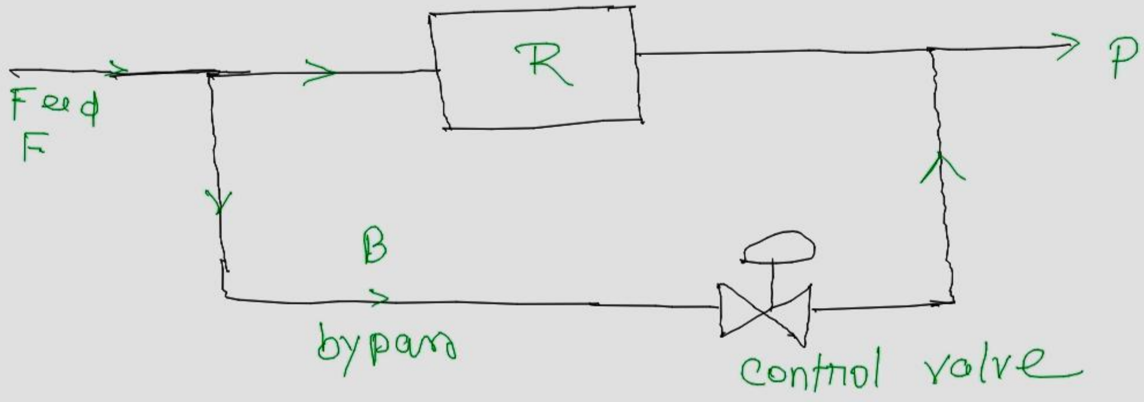
→ component material balance for unit process

(in + generation) − (out + disapperance) = accumulation

due to chemical rxn generation of product and disappearance of reactant terms will come under consideration

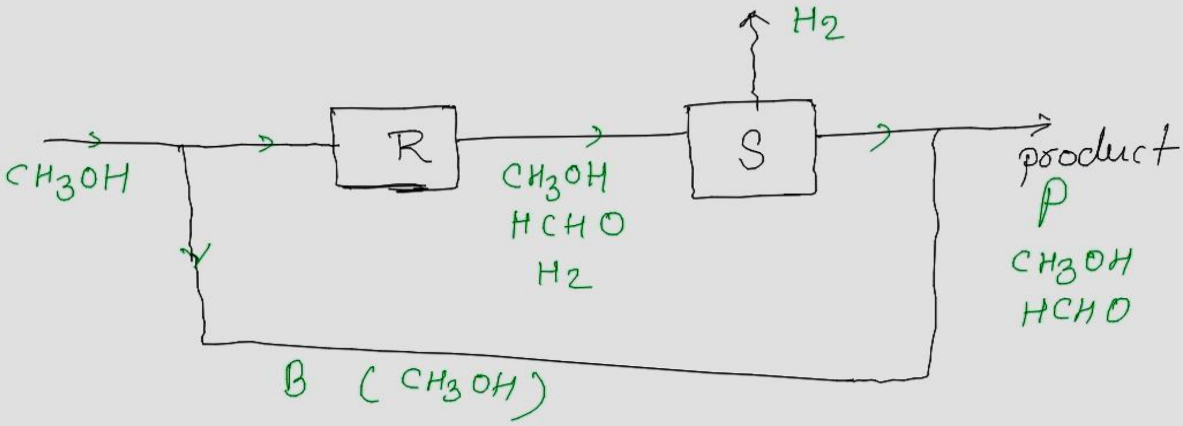
Reactor with bypass —

- purpose of bypass is to control the product specification and conversion of the reactor.



- Control valve is used for controlling the flow rate of bypass stream

Example —



$$CH_3OH \longrightarrow HCHO + H_2$$

given —

- product contains 30% HCHO and 70% CH_3OH
- Single pass conversion of reactor = 50%

find —

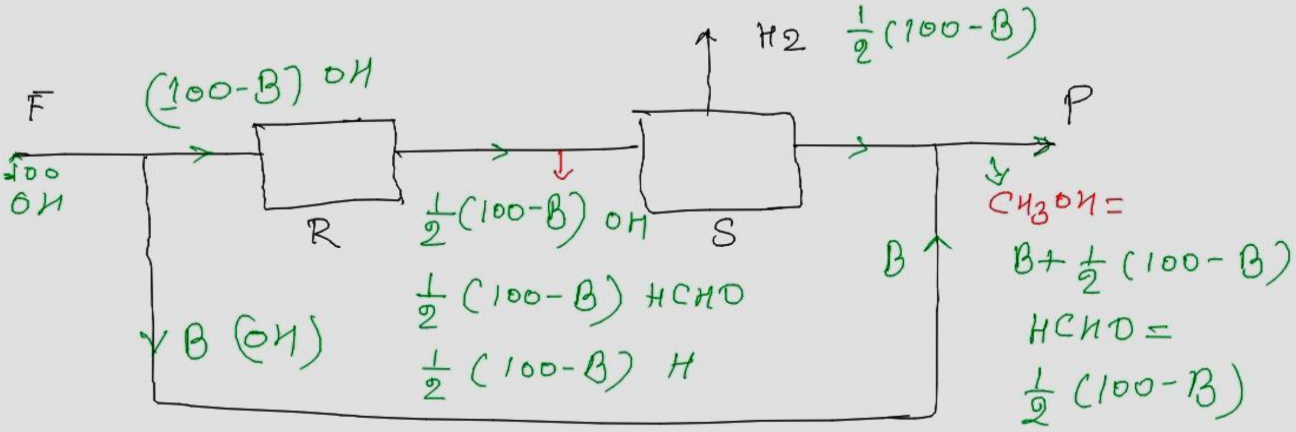
B / F (bypass to feed ratio)

H_2 formed per mol CH_3OH feed —

Solution

basis : CH_3OH feed 100 mol/hr

CH_3OH fed to reactor = 100 - B



CH_3OH at the outlet of Reactor —

$\frac{1}{2}(100 - B)$ [50% conversion

HCHO at the outlet of Reactor —

$\frac{1}{2}(100 - B)$

product will contain $\frac{1}{2}(100 - B)$ HCHO

unreacted CH_3OH will be mixed with bypass stream .

hence product will contain

$B + \frac{1}{2}(100 - B)$ CH_3OH

product is 30% HCHO —

$$\frac{\left[\frac{1}{2}(100-B)\right]}{\left[B + \frac{1}{2}(100-B)\right] + \left[\frac{1}{2}(100-B)\right]} = 0.30$$

$B = 40$

→ $\frac{B}{F} = \frac{40}{100} = 0.4$ Ans

→ HCHO formed $\frac{1}{2}(100 - B) = 30$

HCHO formed per mol of feed $= \frac{30}{100}$

$= 0.30$ Ans

Example —

- A gas mixture contain (20% CO_2, 50% CO and 30% N_2).
- CO_2 is completely absorbed in absorption column and remaining gas stored in 50 m^3 tank at 1atm & 30°C.
- N_2 introduced to the tank to reduce CO concentration upto 20%. N_2 is at

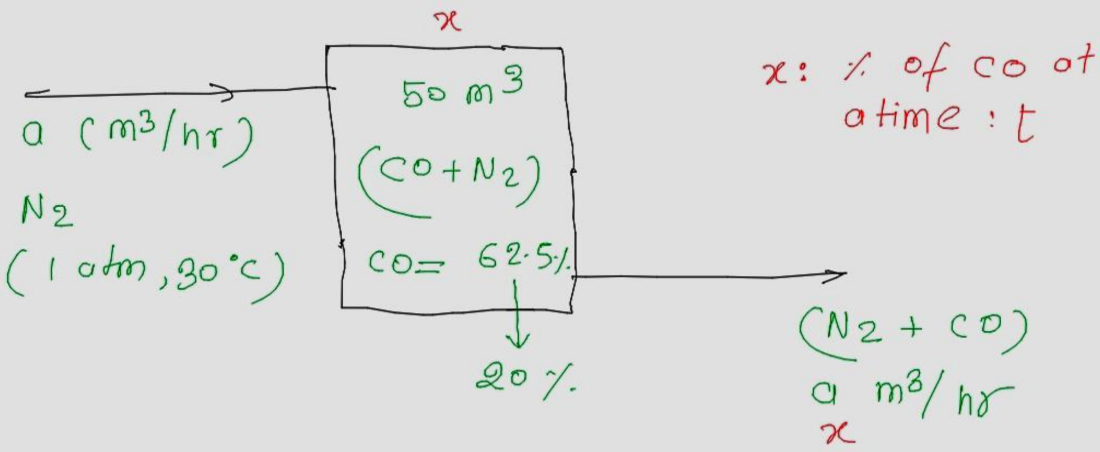
1 atm & 30°C. what is the molar flow rate of N_2 (Mol/sec) required to reduce CO concentration in 1 hr.

- Volumetric inlet of N_2 is equal to the total volumetric flow rate of outlet.

Solution :- material balance of CO

CO: in − out = accumulation

Let inlet and outlet flow rate = a m^3/hr



CO: in − out = accumulation

$$0 - \rho a x = \frac{d(50 x \rho)}{dt}$$

$$-a\,dt = 50\,\frac{dx}{x}$$

now initial % CO in tank (as CO_2 absorbed) $= \frac{50}{50+30} \times 100$

$= 62.5$

hence

$$-a\int_{0}^{1} dt = 50\int_{62.5}^{20} \frac{dx}{x}$$

$a = 56.92 \quad m^3/hr$

now molecular flow to be converted into molar flow rate —

$PV = nRT \qquad (1\,atm, 30^\circ C)$

$1.013 \times 10^5 \times 56.52 = \dot{n} \, / \qquad \backslash \, 303$

$\dot{n} = 2272.788 \quad mo \quad hr$

$\dot{n} = 0.631 \quad mol/sec$

Lecture - 13

Energy Balance

- Heat capacity / Enthalphy
- Kopp's Rule
- Heat balance on unit process
- Heat of Reaction
- Hess's Law
- Heat of formation
- Heat of combustion

general Energy balance

E - ra -

+ E dis = ac 'on

Sensitiye heating

$Q = m \quad T$

Cp: heat capacity

heat capacity can be temperature dependent

Latent heating —

$$Q = m\lambda \qquad (\text{phase change})$$

Kopp' Rule —

A + B
C_{pA} , C_{pB}

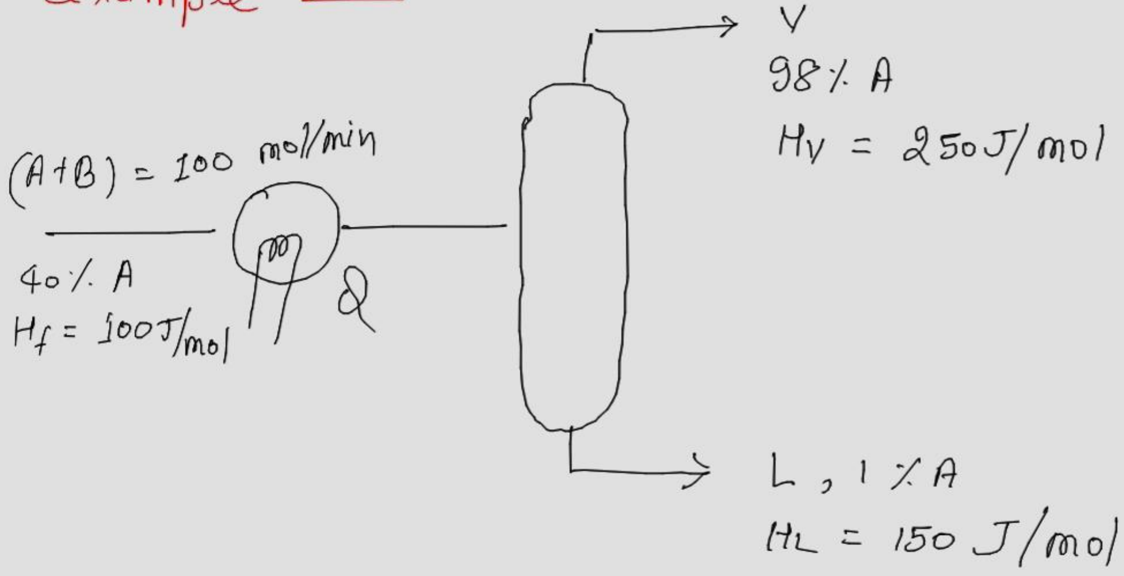
mixture contains two component A & B

heat capacity of mixture

$$\boxed{C_p = x_A C_{pA} + x_B C_{pB}}$$

Energy Balance on unit operation —

Example —



find heat input ~~by~~ heater in watt

Solution —

material balance —

in − out = 0 (steady state)

$100 = L + V$

component $100 \times 0.4 = 0.01 \times L + 0.98 \times V$

$V = 40.20$

$L = 59.79$

Energy balance —

in − out = 0

$(100 \times 100 + Q) = L H_L + V H_V$

$Q = 9018.5$ J/min

$Q = 150.3$ J/sec

Ans

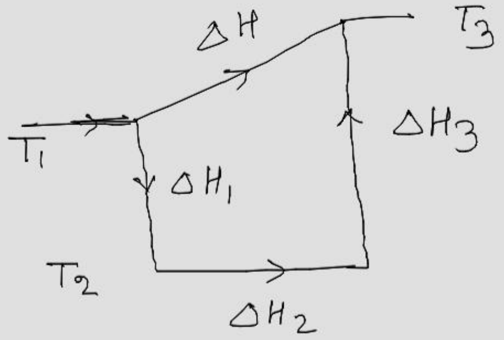
Heat of Reaction —

$A + 2B \longrightarrow C + 3D$ $\Delta H_R = -300$ J/mol

multiply with 2

$2A + 4B \longrightarrow 2C + 6D$ $\Delta H_R = -2 \times 300$ J/mol

Hess' Law —



$$\boxed{\Delta H = \Delta H_1 + \Delta H_2 + \Delta H_3}$$

Heat of formation —

$$\underline{C(s)} + \underline{O_2(g)} \longrightarrow \underline{CO_2(g)} \qquad \underline{\Delta H_R}$$

Standard State of C	Standart state of O_2	Standard state of CO_2

for above rxn enthalphy of rxn will be equal to the heat of formation of CO_2

$$\Delta H_R = \Delta H_f \; CO_2$$

for given rxn —

$$\Delta H_R = \Sigma (v_i \; \Delta H_f)_{product} - \Sigma (n_i \Delta H_f)_{reactant}$$

example :-

$$C_5H_{12} + 5O_2 \longrightarrow 5CO_2 + 6H_2O \qquad \underline{\Delta H_R}$$

$\Delta H_f \; C_5H_{12} = -173$

$\Delta H_f \; H_2O = -393$

$\Delta H_f \; CO_2 = -285.84$

find enthalphy ch

Solution :-

$$\Delta H_R = 5 \times (-285.84) + 6(-393) - (-173)$$

$$= -3614.2$$

Heat of combustion —

$$\Delta H_R = \left(\Sigma \nu_i \Delta H_{ci}\right)_{reactant} - \left(\Sigma n_i \Delta H_{ci}\right)_{product}$$

Lecture - 14

Energy Balance - 02

- flame temperature
- Adiabatic flame temperature
- Net calorific Value
- Gross calorific value

Example .

$CH_4 + H_2O \longrightarrow CO + 3H_2 \qquad \Delta H_R = ?$

given

$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O \qquad \Delta H = -803$

$H_2 + \frac{1}{2}O_2 \longrightarrow H_2O \qquad \Delta H = -242$

$CO + \frac{1}{2}O_2 \longrightarrow CO_2 \qquad \Delta H = -283$

Solution

$CH_4 + H_2O \longrightarrow C \quad 3H_2$

$+2O_2 \downarrow \quad \Delta H_1 = -803$

O_2

$(CO_2 + 2H_2O) + H_2O$

$\downarrow \quad \Delta H_2 = 283$

$(CO + \frac{1}{2}O_2) + 3H_2O$

$\downarrow \quad \Delta H_3 = 3 \times 242$

$(CO + \frac{1}{2}O_2 + 3H_2 + \frac{3}{2}O_2)$

by using Hess's Law –

$$\Delta H = \Delta H_1 + \Delta H_2 + \Delta H_3$$

$$\Delta H = -803 + 283 + 3\times 242$$

$$\Delta H = 206$$

---

flame temperature –

temperature of reaction mixture after completion of exothermic reaction is called flame temperature.

Adiabatic flame temperature –

temperature of reaction mixture after completion of exothermic reaction in a adiabatic reactor is called adiabatic flame temperature.

General Energy balance on combustor –

Energy balance –

To is adiabatic flame temperature

$$\text{in} - \text{out} + \text{generation} = \cancelto{0}{\text{accumulation}}$$

$$\sum \left(m_i \, C_{pi} \, T_i\right) - \sum \left(m_{oi} \, C_{poi} \, T_o\right) + \Delta H = 0$$

$$\boxed{\Delta H = \sum \left(m_o \, C_{po} \, T_o\right) - \sum \left(m_i \, C_{pi} \, T_i\right)}$$

Example —

find adiabatic flame temperature

- CH_4 is burnt with 100 % excess air. air and CH_4 are initially at 25 °C
- specific heat capacity is given below

$C_{p\,O_2}$ = 34.1 J/mol·K

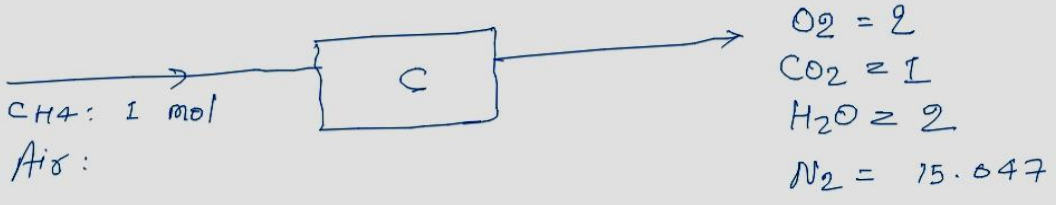
$C_{p\,CO_2}$ = 51.88 ″

$C_{p\,H_2O}$ = 40.45 ″

$C_{p\,N_2}$ = 32.21 ″

basis: 1 mol CH_4

solution — O_2 100 % excess, hence $O_2 = 4$



	CH_4 +	$2O_2$ →	CO_2 +	$2H_2O$
t = 0	1	4	0	0
outlet of Reactor	0	2	1	2

Now energy balance —

$$\left[\Sigma\ m_i C_{pi} (T_i - T_r)\right] - \left[\Sigma\ m_o C_{po} (T_o - T_r)\right]$$

$$+ 8 \times 10^5 = 0$$

T_r : reference temeperature —

suppose reference temperature = 25 °C

hence $\left[\Sigma\ m_i C_{pi} (T_i - T_r)\right] = 0$

$$8 \times 10^5 = \Sigma\ m_o C_{po} (1 \quad 1_r)$$

$$8 \times 10^5 = (2 \times 34.1 + 51.88 \times 1 \quad 40.45 \times 2 + 15.07$$

$$\times 32.21) \quad 10 - 25)$$

$$T_o = 1196.78\ °C$$

outlet temperature is adiabatic flame femerature = 1196.78 °C

$\frac{\text{Air}}{\text{fuel}}$ ratio increases then, adiabatic flame temperature will reduce

Example

CO & pure O_2 burnt in a combustor initially at 25°C. Heat loss in combustor is 15 KJ/mol CO. flame temperature 2125 °C.

given –

$C_{pO_2} = 25 + 14 \times 10^{-3} T$

$C_{pCO_2} = 25 + 42 \times 10^{-3} T$

$\Delta H_f \; CO_2 = -390 \;\; J/mol$

$\Delta H_f \; CO = -110 \;\; J/mol$

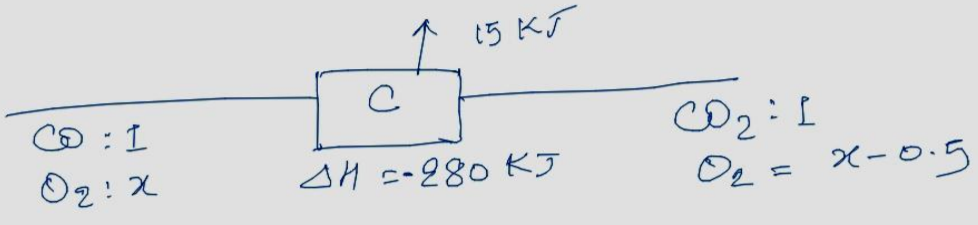
find excess oxygen used = ?

Solution –

heat of Reaction $CO + \frac{1}{2} O_2 \rightarrow CO_2$

$$\Delta H_R = (-390) - (-110) = -280 \;\; KJ/mol$$

basis = 1 mol CO , x mol O_2



CO	$+$	$\frac{1}{2} O_2$	$\longrightarrow$	CO_2
1		x		0
0		$(x-0.5)$		1

hence $(280-15) \times 10^3$ J energy will be used ~~to~~ to raise temperature of rxn mixture —

$$(280-15) \times 10^3 = \sum \int_{298}^{2398} (m\,C_p\,dT)$$

$$265 \times 10^3 = \int_{298}^{2398} (25 + 42 \times 10^{-3} T)\, dT$$

$$+ \int_{298}^{2398} (x - 0.5)(25 + 14 \times 10^{-3} T)\, dT$$

$$\underline{x = 1.53}$$

supplied O_2 = 1.53

required O_2 = 0.5

$$\% \text{ excess} = \frac{1.53 - 0.5}{0.5} \times 100$$

$$= 206\ \%\ \text{excess}$$

Ans

Net Calorific Value –

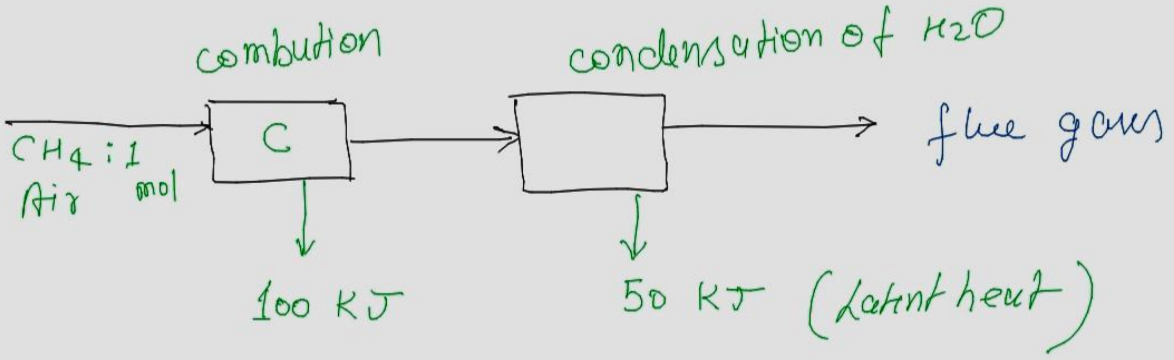
Energy produced by a fuel when it is burnt completly.

NCV unit ⇒ KJ/Kg

KJ/ Kmol

Gross Calorific Value –

$$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$$



Gross calorific value = Net calorific value + latent energy of H_2O

$$\boxed{GCV > NCV}$$