



India's Best Institute for CHEMICAL ENGINEERING

**CHEMICAL ENGINEERING**

REVISED AS PER GATE

# PROCESS CALCULATIONS





# CHEMICAL ENGINEERING

Revised as Per New Gate Syllabus

STUDY MATERIAL

PROCESS CALCULATIONS

**GATE-2024 Syllabus: Chemical Engineering - CH**

**Process Calculations:** Steady and unsteady state mass and energy balances including multiphase, multi-component, reacting and non-reacting systems. Use of tie components; recycle, bypass and purge calculations; Gibb's phase rule and degree of freedom analysis.

**Process Calculations-PC****Marking Analysis in GATE (2010 to 2024)**

Year	1 Mark	2 Marks	Total Marks
2024	1 × 1	2 × 2	5
2023	1 × 1	2 × 2	5
2022	1 × 0	2 × 2	4
2021	1 × 1	2 × 1	3
2020	1 × 0	2 × 2	4
2019	1 × 0	2 × 1	2
2018	1 × 2	2 × 0	2
2017	1 × 0	2 × 1	2
2016	1 × 1	2 × 2	5
2015	1 × 0	2 × 1	2
2014	1 × 0	2 × 2	4
2013	1 × 0	2 × 2	4
2012	1 × 0	2 × 3	6
2011	1 × 0	2 × 2	4
2010	1 × 0	2 × 2	4

**List of Topics in GATE 2024 paper from Process Calculations**

**(Degree of freedom)+ Recycle reactor)+(Energy balance).**

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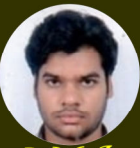







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and many more ....

## CHAPTER-1

## INTRODUCTION

**Units & Dimensions**

- (1.) **Newton (N):** The SI unit of force. It is equal to the force that would give a mass of one kilogram an acceleration of one  $\text{m/s}^2$ , and is equivalent to 100,000 dynes.

Metric unit of force, used also as a unit of weight (force due to gravity).

$$1 \text{ Newton} = 1 \text{ kg} \cdot \text{m/s}^2$$

The definition of the standard metric unit of force is stated by the above equation. One Newton is defined as the amount of force required to give a 1-kg mass an acceleration of  $1 \text{ m/s}^2$ .

- (2.) **Kilogram-force ( $\text{kg}_f$ ):** The **kilogram-force** is a metric unit of force ( $\text{kgf}$ ). The kilogram-force is equal to a mass of one kilogram multiplied by the standard acceleration due to gravity on Earth, which is defined as exactly 9.80665 meter per second<sup>2</sup>. Then one (1) kilogram-force is equal to  $1 \text{ kg} \times 9.80665 \text{ meter per second}^2 = 9.80665 \text{ kilogram} \times \text{meter per second}^2 = 9.80665 \text{ newton (1N)}$ .

**Note :** A kilogram-force ( $\text{kgf}$ ), also called kilopond ( $\text{kp}$ ), is a gravitational metric unit of force.

- (3.) **Mole:** Mole is a unit of measurement used in **chemistry** to express amounts of a **chemical** substance, defined as the amount of any substance that contains as many elementary entities as there are atoms in 12 grams of pure carbon-12, the isotope of carbon with relative atomic mass of exactly 12 by definition.

In other words a **mole** is simply a unit of measurement. Units are invented when existing units are inadequate. Chemical reactions often take place at levels where using grams wouldn't make sense, yet using absolute numbers of atoms/molecules/ions would be confusing, too.

A mole is the quantity of anything that has the same number of particles found in 12.000 grams of carbon-12. That number of particles is Avogadro's Number, which is roughly  $6.02 \times 10^{23}$ . A mole of carbon atoms is  $6.02 \times 10^{23}$  carbon atoms. A mole of chemistry teachers is  $6.02 \times 10^{23}$  chemistry teachers.

**Examples:** 1 mole of  $\text{NH}_3$  has  $6.022 \times 10^{23}$  molecules and weighs about 17 grams. 1 mole of copper has  $6.022 \times 10^{23}$  atoms and weighs about 63.54 grams.

$$\text{Mole} = \frac{\text{mass in gram}}{\text{molecular weight}}$$

- (4.) **Avogadro's number:** Avogadro's number is the number of particles found in one mole of a substance. It is the number of atoms in exactly 12 grams of carbon-12. This experimentally determined value is approximately  $6.022 \times 10^{23}$  particles per mole. Also known as Avogadro's constant

$$1\text{mol}=6.023\times 10^{23}\text{atoms}$$

- (5.) **Pressure:** The ratio of force to the area over which that force is distributed. Pressure is force per unit area applied in a direction perpendicular to the surface of an object.

$$P = \frac{\text{Force}}{\text{Area}} = \frac{F}{A} = \frac{F \cdot d}{A \cdot d} = \frac{W}{V} = \frac{\text{Energy}}{\text{Volume}}$$

- (6.) **Gauge pressure:** The amount by which the pressure measured in a fluid exceeds that of the atmosphere. Gauge pressure is the pressure relative to atmospheric pressure. Gauge pressure is positive for pressures above atmospheric pressure, and negative for pressures below it.

$$\text{Absolute pressure} = \text{Gauge pressure} + \text{Atmospheric pressure}$$

- (7.) **Absolute pressure** is zero-referenced against a perfect vacuum, so it is equal to gauge pressure plus atmospheric pressure. A barometer is a device that measures atmospheric pressure.

- (8.) **Vacuum pressure** - Pressures below atmospheric pressure are called vacuum pressures and are measured by vacuum gages that indicate the difference between the atmospheric pressure and the absolute pressure.

$$P_{\text{gauge}} = P_{\text{absolute}} - P_{\text{atmospheric}}$$

$$P_{\text{vacuum}} = P_{\text{atmospheric}} - P_{\text{absolute}}$$

$$P_{\text{absolute}} = P_{\text{atmospheric}} + P_{\text{gauge}}$$

- (9.) **Molarity (M):** Molarity's definition is a unit of measurement used to denote the concentration of a particular substance or solution. Molarity is expressed as moles of solute over liters of solution. It is denoted either by a capital M or by the term molar.

$$\text{Molarity (M)} = \frac{\text{No. of gram moles of solute}}{\text{Volume of solution in Litre}}$$

- (10.) **Normality(N):** Normality is a measure of concentration equal to the gram equivalent weight per liter of solution. Gram equivalent weight is the measure of the reactive capacity of a molecule.

$$\text{Normality (N)} = \frac{\text{Gram equivalent of solute}}{\text{Volume of solution in Litre}}$$

For acid reactions, a 1 M H<sub>2</sub>SO<sub>4</sub> solution will have normality (N) of 2 N because 2 moles of H<sup>+</sup> ions are present per liter of solution. For sulfide precipitation reactions, where the SO<sub>4</sub><sup>-</sup> ion is the important part, the same 1 M H<sub>2</sub>SO<sub>4</sub> solution will have a normality of 1 N.

- (11.) **Molality:** Molality is the number of moles of solute per kilogram of solvent. It is important the mass of solvent is used and not the mass of the solution. Solutions labeled with molal concentration are denoted with a lower case m.

$$\text{Molality (m)} = \frac{\text{No. of gram moles of solute}}{\text{Weight of solvent in Kilogram}}$$

## KEY POINTS TO REMEMBER

**(Introduction)**

- (1.)  $\text{Mole} = \frac{\text{mass in gram}}{\text{molecular weight}}$
- (2.)  $1 \text{ mole} = 6.023 \times 10^{23} \text{ atoms}$
- (3.) **Absolute pressure** = gauge pressure + atmospheric pressure
- (4.) **Absolute pressure** = atmospheric pressure – vacuum
- (5.) **Ideal gas equation**  $\Rightarrow$   $PV=nRT$   
Where P = Absolute pressure
- (6.) **Boyle's law:**  $PV=\text{constant}$   
V = Volume occupied by gas
- (7.) **CHARLES's Law:**  $-\frac{V}{T}=\text{constant}$  where T = Absolute temperature
- (8.) **Gas density** =  $\frac{\text{molecular weight of gas}}{\text{molal volume of gas}}$
- (9.) **Specific gravity of gas** =  $\frac{\text{molecular weight of gas}}{\text{molal weight of air}}$
- (10.) **pH** =  $-\log_{10} (H^+)$
- (11.) **Compressibility factor:**  $Z = \frac{PV}{nRT}$



## NUMERICALS

**Question-1:** A compound whose molecular weight is 106, & composition on weight basis  
 C – 85%      H<sub>2</sub> – 5%      N<sub>2</sub> – 10%  
 Find formula of this compound.

**Solution:** Basis: compound is 106 kg (1 kg mol)  
 Carbon amount =  $\frac{85 \times 106}{100} = 90.1 \text{ kg}$   
 kg atoms of carbon =  $\frac{90.1}{12} = 7.51 \simeq 8$   
 Amount of hydrogen =  $\frac{5 \times 106}{100} = 5.3$   
 kg atoms of hydrogen =  $\frac{5.3}{1} = 5.3 \simeq 5$   
 Nitrogen amount =  $\frac{10 \times 106}{100} = 10.6$   
 kg atoms of nitrogen =  $\sum$   
 Hence, the compound formula is given by:  $\boxed{\text{C}_8\text{H}_5\text{N}}$

**Question-2:** If a gas mixture contain 0.0255 mol. Calculate the mixture density in gram per liter at 30°C and 750 mm Hg

**Solution:** Assuming gas follows ideal gas law  
 $\boxed{PV = nRT}$   
 $n = 0.0255 \text{ mol}, \quad T = 30 + 273 = 303 \text{ k}$   
 $R = 62.4 \frac{(\text{mm. Hg})(\text{lit})}{(\text{gm. mol})\text{k}}$   
 $V = \frac{nRT}{P} = \frac{0.0255 \times 62.4 \times 303}{750} = 0.567 \text{ lit}$   
 Mixture density =  $\frac{1}{0.567} = 1.76 \text{ gm/liter}$

**Question-3:** The concentration of SO<sub>2</sub> in the flue gases from a boiler was found to be 0.2 kg/ m<sup>3</sup> at NTP. Determine the concentration of SO<sub>2</sub> in parts per million at NTP. Assume that the flue gases are perfect.

**Solution:** We know for a perfect gas at NTP  
 1 kmol = 22.4 m<sup>3</sup>  
 Molecular weight of SO<sub>2</sub> = (32 + 2 × 16) = 64 kg/kmol  
 $0.2 \text{ kg/m}^3 \text{ of SO}_2 = \frac{0.2}{64} = 3.125 \times 10^{-3} \text{ kmol/m}^3$   
 Hence for NTP case,  
 $3.125 \times 10^{-3} \text{ kmol/m}^3 = 3.125 \times 10^{-3} \times 22.4$   
 $= 0.07 \text{ m}^3/\text{m}^3$   
 $= 0.07 \times 10^6 \text{ PPM} = 70000 \text{ ppm}$

**Question-4:** Calculate the volume occupied by 1 gm mole of water vapor at 900° C and 100 atm.

(i) By the perfect gas law

(ii) Using Vander Waal's equation

The Vander Waal's constants for water are :

$$a = 5.404 \text{ (litre)}^2 \text{ atm/ (gm.mol)}^2$$

$$b = 0.3049 \text{ litre/ (gm.mol)}$$

$$\text{Vander Waal's equation } \left( P + \frac{a}{V^2} \right) (V - b) = RT$$

**Sol.**  $R = 0.082 \text{ litre-atm/ (gm.mol) (}^\circ\text{K)}$

$$T = 1173 \text{ K, } P = 100 \text{ atm } n = 1.0 \text{ gm mol}$$

$$(a) \quad V = \frac{nRT}{P} = \frac{0.082 \times 1173}{100} = 0.963 \text{ lit}$$

$$(b) \quad \left( P + \frac{a}{V^2} \right) (V - b) = RT = 0.082 \times 1173 = 96.3$$

$$\text{or } \left( 100 + \frac{5.404}{V^2} \right) (V - 0.3049) = 96.3$$

By solving  $V = 0.94 \text{ litre}$

$$\text{Dry flues gas (H}_2\text{O free) having CO}_2 \text{ percentage} = \frac{1}{1 + 2.6 + 17.3} \times 100 = 4.78\%$$

The percentage of CO<sub>2</sub> in the flue gas is much lower than the specific limit (*i.e.*, 15%)

So, the charge of the inspector against the factory is not correct.

## CHAPTER-2

## MATERIAL BALANCE CALCULATION

**Introduction:**

- Material balance calculations are the basis for process design.
- A material balance can decide product and raw material quantity.
- Material balance can be applied in numerous ways:
  - Overall material balance.
  - Component material balance
  - Species material balance (eg C, H, O etc.)
  - Material balance can be applied over a single process unit, set of process units or for the whole plant.
- Material balance calculations sets the composition and process system flow rates.
- Material balance are important tools to
  - Trouble shooting study
  - Check design performance.
  - Locate source of material loss.
  - Check instrumentation calibrations.

**General Material Balance:**

- Material Balances are nothing more than the application of the “law of conservation of mass” i.e. “Matter is neither created nor destroyed”.
- Material balance problems are much easier if we develop a systematic strategy.
- General material balance equation is given by
 
$$\sum[\text{Input to the system}] - \sum[\text{output from the system}] + [\text{Generation in the system}] - [\text{consumption in the system}] = [\text{Accumulation in the system}]$$
- For steady state process accumulation term becomes zero.
- In case if there is no chemical rxn then generation and consumption terms also becomes zero.
- For steady state case and no chemical rxn the generalised equation becomes.
 
$$\sum[\text{Input to the system}] = \sum[\text{output to the system}]$$
- The generalised chemical equation can be applied to conservation of total mass, mass of a component, moles of a component, mass of an atomic species, moles of an atomic species, but not to volume (because different materials have different densities)

**Composition Measurement:**

1. If  $n_i$  be the number of moles of individual chemical species  $i$  in the mixture and  $n$  be the total number of moles of the given mixture, then mole fraction for species  $i$  is given by

$$x_i = \frac{n_i}{n}$$

2. Molar concentration is defined as the ratio of mole fraction  $i$  to its molar volume.

3. Mathematically molar concentration is given by  $c_i = \frac{x_i}{v}$

Where:  $c_i$  = molar concentration of chemical species  $i$ .

$v$  = molar volume

$x_i$  = mole fraction of species  $i$ .

### Characteristics of Systems:

- Any arbitrary portion or a whole process considered for analysis is called a system.
- If no mass exchange occurs with the surroundings then system is called closed system.
- If mass exchange occurs with the surrounding or material crosses the system boundary than system is called open system.
- If in a system, a variable, such as an amount of material or a property does not changes with time then this state of a system is called steady state.
- For steady state system accumulation term is always zero.
- If a variable or any property of the system changes with time then this is unsteady state system.
- A continuous process is one in which material enters and leaves the system without interruption.
- A batch process is one, which is a closed system, treats a fixed amount of material each time it operates.
- In a semi-batch process, which is an open process, material enters the process during its operation but none leaves.

### Material Balance Calculations:

- For multi component systems, a seprate material balance equation for each component can be written plus one additional material balance equation based on the total mass of the system, but one set will be dependent.
- For solving material balance equation following steps needs to be followed :
  - i) Choose a basis
  - ii) Determine the number of variables whose values are unknown.
  - iii) Determine the number of independent equations and carry out a degree of freedom analysis.

Types of equation:

- a) Independent material balance equations as many as species involved in the systems.
  - b) The basis
  - c) Explicit relations: Specified in the problem statement such as product to feed ratio.
  - d) Implicit relations: Particularly the sum of the mass or mole fraction in a stream being unity.
- iv) Once the number of unknowns and independent equation are determined, then the degree of freedom analysis are can be done to determine whether a problem is solvable or not.

Let  $N_D$  – Degrees of freedom.

$N_U$  – Number of unknowns.

$N_E$  – Number of independent equation.

$$N_D = N_u - N_E$$

Cases:	$N_D$	
(a) $N_u = N_E$	0	Exactly specified a solution exists.
(b) $N_u - N_E > 0$	$> 0$	Underspecified; more independent equation required
(c) $N_u - N_E < 0$	$< 0$	Over specified; in general no solution exist unless some constraints are eliminated.
v)		Write down the equation to be solved in terms of the knowns and unknowns.
vi)		Solve the equations and calculate the quantities asked for in the problems.

**Stoichiometry:**

- Stoichiometry provides a quantitative means of relating the amount of products produced by a chemical reactions to the amount of reactants or vice-versa.
- Chemical reaction equation tells what substance are reactants and what substance are products.
- The coefficients of a balanced chemical reaction tells what the mole ratios are among the substances that react or are produced.
- Steps to be followed for solving problems involving stoichiometry.
  - Chemical equation should be correctly balanced.
  - Proper degree of completion for the reaction should be used.
  - Molecular weights are used to convert mass to moles for the reactants and moles to mass for the products.
  - Coefficients in the chemical equation should be used to obtain the relative molar amounts of product produced and reactant consumed in the reaction.
- Consider a general chemical reaction equation
 
$$cC + dD \rightleftharpoons aA + bB \quad \dots(1)$$
 Equation (1) can also be written as
 
$$v_A A + v_B B + v_C C + v_D D = \sum_1 v_i S_i = 0$$
  - Where  $v_i$  is the stoichiometric coefficient for species  $S_i$ .
  - The products are defined to have positive values for stoichiometric coefficients and the reactants to have negative values.
  - The ratio of stoichiometric coefficients are unique for a given reaction.
 
$$v_c = -c \quad v_A = a$$

$$v_d = -d \quad v_B = b$$

**Extent of Reaction**

- Extent of reaction,  $\xi$  is based on a specified stoichiometric equation and denotes how much reaction occurs.
- The extent of reaction is calculated by dividing the change in the number of moles of a species that occurs in a reaction, for either a reactant or a product by the associated stoichiometric coefficients.

$$\xi = \frac{n_i - n_{i0}}{v_i}$$

Where:  $n_i \rightarrow$  moles of species  $i$  present in the system after the reaction.

$n_{i0} \rightarrow$  moles of species  $i$  present in the system when the reaction starts.

$v_i \rightarrow$  stoichiometric coefficients for the species  $i$  in the specified chemical reaction equation.

$\xi \rightarrow$  extent of reaction.

→ negative, denotes consumption.

if  $(n_i - n_{i0}) \rightarrow$  positive, denotes generation.

### Limiting and Excess Reactants:

- If a chemical reaction proceeds to completion, then the species present in the chemical reaction that would be the first to be completely consumed is called limiting reactant.
- All the reactants other than limiting reactant are called excess reactant.
- Maximum extent of reaction is calculated by assuming complete reaction. The reactant with smallest maximum extent of reaction is the limiting reactant.
- Conversion is the fraction of the limiting reactant in the feed that is converted into products.

$$\% \text{ conversion} = 100 \times \frac{\text{moles of the limiting reactant in the feed that reacts.}}{\text{moles of the limiting reactant introduced in the feed.}}$$

or

$$\text{Conversion} = \frac{\text{extent of reaction that actually occurs}}{\text{extent of reaction that would occur if complete reaction took place.}} = \frac{\xi}{\xi_{\max.}}$$

### Selectivity and Yield.

- Selectivity is the ratio of the moles of a desired product to the moles of undesired or by product.
- Selectivity is helpful in determining the product quantity w.r.t. reactants.
- For the process to be economical, the value of product has to be greater than the value of the reactants.
- Yield is defined on three basis:

$$(a) \text{ Yield (based on feed)} = \frac{\text{amount of desired product.}}{\text{amount of key reactant consumed.}}$$

$$(b) \text{ Yield (based on 100\% conversion)} = \frac{\text{amount of product obtained}}{\text{amount of key reactant consumed}}$$

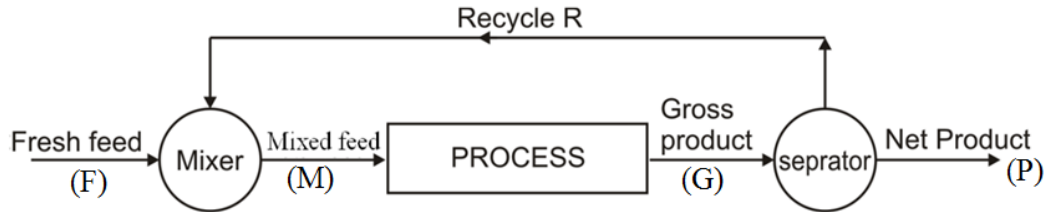
$$(c) \text{ Yield (based on 100\% conversion)} \\ = \frac{\text{amount of product obtained}}{\text{amount of product obtained theoretically based on limiting reactant.}}$$

Key reactant is generally limiting reactant.

- Because of the presence of impurities side reactions, reversible reactions; yield in reaction is not equal to theoretical yield.

### Recycle systems:

- Recycling is a process in which unused feed is taken back from a downstream unit to the upstream unit.
- Recycling is very important, where the cost of raw materials are very high.
- Recycle of unused reactant to the reactor can offer significant economic savings for high-volume processing systems.
- Recycle is very common in many chemical process such as distillation, crystallization, refrigeration and heating.



- The most common application of recycle for systems involving chemical reaction is the recycle of reactants, an application that is used to increase the overall conversion in a reactor.

$$\text{Overall conversion } (f_{OA}) = \frac{\text{amount of fresh feed} - \text{amount of net product}}{\text{amount of fresh feed}}$$

$$\text{Single-pass conversion } (f_{SP}) = \frac{\text{amount of mixed feed} - \text{amount of gross product}}{\text{amount of mixed feed}}$$

- $f_{OA}$  is based on overall process.  $f_{SP}$  is based on a particular reactor.
- Extent of reactant is the same regard less of whether an overall material balance is used or a material balance for the reactor is used.
- Some useful correlations:**

$$(i) \quad \xi = \frac{(-f) \eta_{\text{limiting reactant}}^{in}}{v_{\text{limiting reactant}}}$$

$$\text{Let } \eta_{\text{limiting reactant}}^{in} = \eta_{LR}^{FF}$$

$$v_{\text{limiting reactant}} = v_{LR}$$

Overall conversion for the limiting reactant

$$f_{OA} = \frac{-v_{LR} \xi}{\eta_{LR}^{FF}}$$

Single-pass conversion =  $f_{SP}$

$$f_{SP} = \frac{-v_{LR} \xi}{\eta_{LR}^{RF}}$$

Mixing point = Fresh feed + Recycle feed.

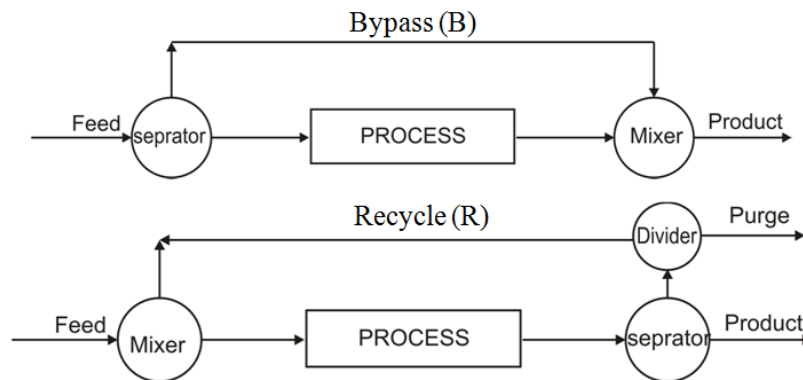
$$\eta_{LR}^{RF} = \eta_{LR}^{FF} + \eta_{LR}^{recycle}$$

Relationship between overall and single pass conversion is given by (or it can be obtained by using above relations)

$$\frac{f_{SP}}{f_{OA}} = \frac{\eta_{LR}^{FF}}{\eta_{LR}^{FF} + \eta_{LR}^{recycle}}$$

**Bypass and Purge:**

- 1.(i) Bypass stream is the one that skips one or more stages of the process and goes directly to another downstream process.
- (ii) Bypass stream is used to maintain the composition and temperature in the process.
- 2.(i) Purge stream is a stream which is bled off from the process to remove an accumulation of inerts or unwanted material that might otherwise build up in the recycle stream with time of operation.



- (ii) If inerts are not removed through purge stream then they will go on accumulating until the process no longer function properly.
- (iii) An example of purge stream are distillation coloumn which without an overhead purge and with light trace impurity in the feed will experience a steady increase in coloumn pressure which will ultimately results in reduction in separation performance.

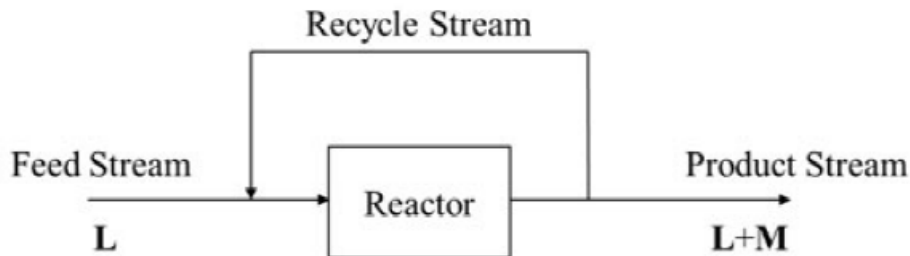


## KEY POINTS TO REMEMBER

- (1.) General mass balance equation is given by—  
Mass in + mass generated = mass out + mass consumed + accumulation
- (2.) In case of steady state rate of accumulation is zero whereas in case of unsteady state operation rate of accumulation is not zero.
- (3.) **Mass fraction**  $x_i = \frac{n_i}{n}$
- (4.) **Molar concentration**  $c_i = \frac{x_i}{V}$   
Where V = molar volume
- (5.) **Conversion** =  $\frac{\text{amount of reactant consumed}}{\text{amount of reactant supplied}}$
- (6.) **Yield** =  $\frac{(\text{moles of product formed})(\text{stoichiometric factor})}{\text{moles of reactant converted}}$
- (7.) **Overall fractional conversion**  
$$E = E_0 \times \exp \left[ \left( \frac{L}{R_v} \right) \times \left\{ \left( \frac{1}{T_0} \right) - \left( \frac{1}{T_d} \right) \right\} \right]$$
 and  
$$E_s = E_0 \times \exp \left[ \left( \frac{L}{R_v} \right) \times \left\{ \left( \frac{1}{T_0} \right) - \left( \frac{1}{T} \right) \right\} \right]$$
- (8.) **Batch process:** A process in which material is neither added nor removed from a process during its operation.
- (9.) **Closed system:** A system that does not have material crossing the system boundary.
- (10.) **Continuous process:** A process in which material enter/or exits continuously.
- (11.) **Degree of freedom:** The no. of variables whose values are unknown minus the number of independent equations.
- (12.) **Implicit equation:** An equation based on information not explicitly provided in a problem such as sum of mass fraction is 1.
- (13.) **Negative accumulation:** A depletion of material in a system.
- (14.) **Semi – batch process:** A process in which material enters the system but product is not removed during operations.
- (15.) **Transient system** – Unsteady state system.
- (16.) **Tie component:** A component that enters a process in only one stream and leaves in only stream and does not react inside the process.
- (17.) **Degree of completion:** Fraction of the limiting reactant converted to products.
- (18.) **Limiting reactant** – The species in a chemical reaction that would theoretically run out first if the reaction were to proceed to completion according to the chemical equation.
- (19.) **Excess reactant** – All reactants other than limiting reactant.
- (20.) **Bypass stream** – A stream that skips one or more units of a process and goes directly to a downstream unit.
- (21.) **Once through fraction conversion** – The conversion of a reactant based on the amount of material that material enters or leaves a reactor.
- (22.) **Overall fraction conversion** – Conversion of a reactant with recycle included.
- (23.) **Purge:** A stream bled off from a process to remove the accumulation of inert or impurities that might otherwise build up in the recycle stream.

## NUMERICAL

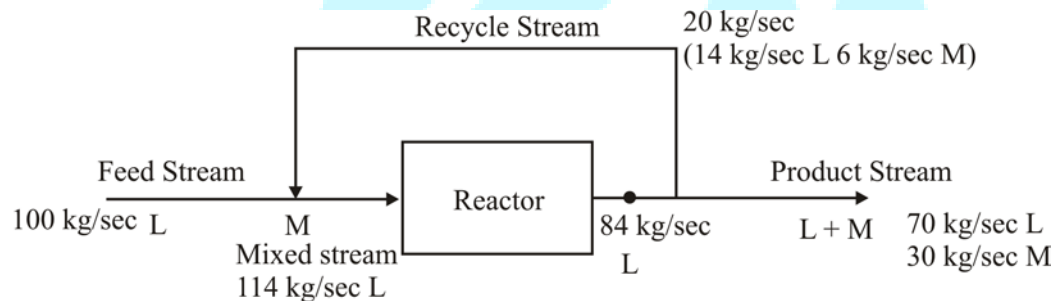
**Question-01:** A feed stream containing pure species L flows into a reactor, where L is partly converted to M as shown in the figure  
(GATE-2020 2-Marks)



The mass flow rate of the recycle stream is 20% of that of the product stream. The overall conversion of L (based on mass units) in the process is 30%. Assuming steady state operation, the one-pass conversion of L (based on mass units) through the reactor is \_\_\_\_\_

- (a) 23.8%                      (b) 26.3%                      (c) 30%                      (d) 34.2%

**Answer: B**



Let mass flow rate of feed = 100 kg / sec

$$\therefore \quad \% \text{ single pass conversion of L, } x_L = \frac{114 - 84}{114} \times 100 = 26.31$$

**Question-02:** A tank initially contains a gas mixture with 21 mol% oxygen and 79 mol% nitrogen. Pure nitrogen enters the tank, and a gas mixture of nitrogen and oxygen exits the tank. The molar flow rate of both the inlet and exit streams is  $8 \text{ mol s}^{-1}$ .

In addition, use the following data and assumptions

- Assume the tank contents to be well mixed

## CHAPTER-3

## ENERGY BALANCES CALCULATIONS

**Terms involved in Energy Balances**

- 1) **Heat:** It is defined as a form of energy that flows across the system boundary which is caused by a temperature difference between the system and surroundings.
  - It is denoted by Q.
  - Heat is positive when transferred to the system and negative when removed from the system.
  - Heat is a path variable
  - $Q = UA (T_2 - T_1)$   
Where: U – Overall heat transfer coefficient  
A – Area for heat transfer.  
 $T_2 - T_1$  – Temperature difference.
- 2) **Work:** Work is a form of energy that represents a transfer of energy between the system and surroundings.
  - Work cannot be stored and is a path variable.
  - Work is denoted by W. It is positive when surrounding does work on system and negative when the system performs work on surroundings.
  - Rate of work (i.e. work done per unit time) is power.
  - Work can be any of the form such as mechanical work, electrical work, shaft work, flow work, non flow work etc.
- 3) **Kinetic energy (KE).**
  - Kinetic energy of a material is a macroscopic energy that is associated with the gross movement (velocity) of the system or material
  - K.E is given by
 
$$\boxed{K.E = \frac{1}{2}mv^2}$$
 Where: m: mass, V: velocity of that mass.
  - Specific K.E is K.E per unit mass.  
It is denoted by  $\widehat{K.E}$ . 
$$\boxed{\widehat{K.E} = \frac{1}{2}V^2}$$
  - $\Delta(\widehat{K.E.})$  depends only on final and initial state, so state function.
- 4) **Potential energy (P. E)**
  - PE is a energy stored within the system due to its position above some arbitrary plane.
  - $P.E = mgh$
  - Specific P.E.  $[\widehat{P.E.}] = gh$
  - Here h is measured from the reference level to the centre of mass of the system.

→  $(\Delta P.E.)$  is a state function.

### 5) Flow energy (FE)

→ Flow energy is the energy associated with the fluid element.

→ Whenever a mass of fluid is entered to the system it is being pushed by the force exerted by the fluid behind it to cause some displacement. This force multiplied by displacement of fluid element is called flow energy.

→ Flow energy is given by the work which is equal to PV per unit mass of work done by the flowing fluid.

### 6) Internal Energy (U)

→ Internal energy is a energy associated with molecules, atomic and subatomic species. These species posses K.E due to vibration, rotation and translation.

→ Internal energy can be stored and it is state variable.

→ No absolute value of internal energy exists. Therefore it is calculated by taking some reference.

→ For cyclic and isothermal process change in internal energy is zero.

→ The internal energy of system containing more than one component is given by.

$$U_{\text{tot}} = m_1 \hat{U}_1 + m_2 \hat{U}_2 + \dots + n_n \hat{U}_n$$

whenever  $\hat{U}$  is specific internal energy.

### 7) Enthalpy (H)

→ Enthalpy is a thermodynamic property that measure the heat supplied at constant pressure

→ Enthalpy (H) is given by

$$H = U + PV$$

→  $\hat{H}$  Specific enthalpy for single phase and single component is fixed by two intensive variables i.e. temperature and pressure.

$$\hat{H} = \hat{H}(T, p)$$

$$d\hat{H} = \left( \frac{\partial H}{\partial T} \right)_p dT + \left( \frac{\partial \hat{H}}{\partial p} \right)_T dp \quad \dots(i)$$

First term of equation (i) is the heat capacity at constant pressure and for most practical purposes

$\left( \frac{\partial H}{\partial T} \right)_T dp$  is neglected.

$$\therefore \Delta \hat{H} = \hat{H}_2 - \hat{H}_1 = \int_{H_1}^{H_2} d\hat{H} = \int_{T_1}^{T_2} C_p dT$$

### Important Concepts

→ Enthalpy and internal energy of ideal gases are functions of temperature only.

→ When phase transitions occur (i.e. from solid to liquid) or (liquid to vapour), a large amount of enthalpy changes without any change in temperature. This is called **latent heat**.

→ Change in enthalpy when phase transition occurs from solid to liquid is called **heat of fusion**.

→ Change in enthalpy when phase transition occurs from liquid to vapour is called **heat of vaporization**.

→ Enthalpy changes that takes place within a single phase with change in temperature is called **sensible heat changes**.

## KEY POINTS TO REMEMBER

- 1) **Adiabatic process:** A process in which no heat transfer occurs ( $Q = 0$ )
- 2) **Enthalpy:** The sum of the variables  $U + PV$
- 3) **Path variables** are those whose value depends on how the process takes place such as heat and work.
- 4) **State variable** – value depends only on initial and final state.
- 5) **Latent heat:** An enthalpy change that involves a phase transition.
- 6) **Sensible heat:** An enthalpy change that does not involve phase transition but is due to temperature difference
- 7) **Adiabatic reaction temperature:** Adiabatic reaction temperature or theoretical flame or combustion temperature is the temperature attained by the products when reaction is carried out at adiabatic conditions and limiting reactant heats completely.

## Important Formulae:

- 1) For constant volume process:

$$C_v = \left( \frac{\partial Q}{\partial T} \right)_v = \left( \frac{\partial U}{\partial T} \right)_v$$

- 2) For constant pressure process:

$$C_p = \left( \frac{\partial Q}{\partial T} \right)_p = \left( \frac{\partial H}{\partial T} \right)_p \quad \Delta H = \int_{T_1}^{T_2} C_p \cdot dT$$

where  $C_p$  can be the function of  $T$       ex:  $C_p = a + bT + cT^2$

- 3) Clapeyron equation:

$$\frac{dP^{\text{sat}}}{dT} = \frac{\Delta H_v}{T \Delta V}$$

where:  $P^{\text{sat}}$  – vapour pressure at temp  $T$ ,  $\Delta H_v$  - latent heat of vaporization.

- 4) **Trouton's Rule**  $\frac{\Delta H_{vb}}{T_b} = K$

Where:  $\Delta H_{vb}$  is the heat of vaporization at normal boiling point  $T_b$ .

$K$  is known as Trouton's ratio. Ratio is approximately equal to 87.95/mol-k.

- 5) **Heat of solution:** per mole of solute (component 1) is given by

$$\Delta H_s = \frac{\Delta H}{x_1}$$

Where  $\Delta H$  is heat of mixing  $C_p - C_v = R$

$$\gamma = \frac{C_p}{C_v}$$

- 6) **Bernoulli's equation:**  $\frac{u^2}{2\rho} + gZ + \frac{P}{\rho} = \text{constant}$

**Question-7:** In a laboratory experiment pure methane is burnt with theoretical quantity of air. The part of methane burns but the part that burns goes to  $\text{CO}_2$  and  $\text{H}_2\text{O}$ . If the methane and air are initially at  $25^\circ\text{C}$  and product leaves at  $400^\circ\text{C}$  with water in vapour form what percent of the methane is burnt.

**Data:**

For the oxidation of  $\text{CH}_4$  to  $\text{CO}_2$  and  $\text{H}_2\text{O}$  (vapour) the standard heat of reaction  $\Delta H^\circ_R = 802.9 \text{ KJ/mol}$  of  $\text{CH}_4$  reacted. Specific enthalpies at  $400^\circ\text{C}$  in  $\text{KJ/mol}$  (Reference:

Specific enthalpy at  $25^\circ\text{C} = 0 \text{ KJ/mol}$

$\text{O}_2 = 11.64$

$\text{N}_2 = 11.13$

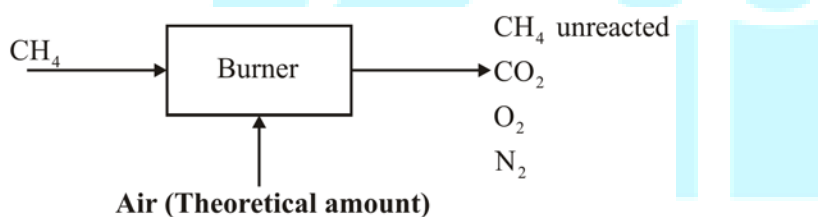
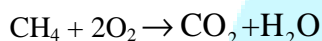
$\text{CH}_4 = 17.22$

$\text{CO}_2 = 16.43$

$\text{H}_2\text{O} = 13.2$

**Solution:**

Basis: 1 mol  $\text{CH}_4$  fed to the burner



Now from energy balance:

Product heat = Reactant heat + heat released from reaction

Since reference temperature is  $25^\circ\text{C}$

Hence, reactant heat = 0

Let,  $a$  be fraction of methane unburnt, then

$$(1 - a)802.9 = 1 \times (1 - a) \times 16.43 + 2 \times (1 - a) \times 13.2 + 2 \times \frac{79}{21} \times 11.13 + 17.22 \times a + 2 \times a \times 11.64$$

On solving  $a = 0.845$

Percentage of methane burnt =  $(1 - a) \times 100 = (1 - 0.845) \times 100 = \mathbf{15.5\%}$

**Question-8:** 1000 kg/hr of a thermic fluid, to be used as a heat transfer medium, is being indirectly heated in a heater from 380 K to 550 K. Calculate the heat load on the heater in kW. Also estimate the mean heat capacity of the thermic fluid over the temperature range of interest. The heat capacity equation for thermic fluid is  $C_p = 1.436 + 0.00218T$  where  $C_p$  is in kJ/kg K and T is in K.

**Solution:** Basis: Thermic fluid has mass flow rate = 1000 kg/hr

$$\text{Now heat load} = m \int_{T_1}^{T_2} C_p dT$$

$$m = 1000 \text{ kg/hr}$$

$$T_1 = 380 \text{ K}, T_2 = 550 \text{ K}$$

$$\text{Hence heat load} = 1000 \int_{380}^{550} (1.436 + 0.00218T) dT = 416449 \text{ kJ/hr}$$

$$C_{p, \text{mean}} = \frac{\int_{T_1}^{T_2} C_p dT}{T_2 - T_1} = \frac{\int_{380}^{550} C_p dT}{550 - 380}$$

$$C_{p, \text{mean}} = \frac{1.436(550 - 380)}{550 - 380} + 0.00218 \times \frac{1}{2} \times \frac{(550^2 - 380^2)}{(550 - 380)}$$

$$= 1.436 + 1.0137 = 2.4497 \text{ kJ/kg K}$$

**Question-9:** The heat of reaction at 300K and at one atmosphere pressure for the following gas phase reaction:  $A + 3B \rightarrow C$  is  $-50,000$  calories per mole of A converted.

Data on the molar heat capacity at constant pressure at (cal/mol-K) of various components are

$$C_p \text{ for A} = -0.4 + 80 \times 10^{-3} T, \quad T \text{ in K}$$

$$C_p \text{ for B} = 7 \quad C_p \text{ for C} = 26$$

Calculate the heat of reaction at 500K and at one atmosphere pressure.

**Solution:** We know that,

$$\text{Reaction heat at 500 K} = [\text{Reaction heat at 300 K} + \text{Product enthalpy} - \text{Reactant enthalpy}]$$

$$= 50,000 + 26(500 - 300) - 3 \times 7(500 - 300) - \left[ (-4)(500 - 300) + 80 \times 10^{-3} \int_{300}^{500} T dT \right]$$

→ On solving we get heat of reaction at 500K =  $-55,320$  calorie /mol A converted

## CHAPTER-4

# COMBUSTION CALCULATIONS

- Combustion is a unit operation.
- Combustion is a process in which oxidation reaction occur.
- Combustion is called complete combustion when combustion product of carbon, hydrogen and sulphur are carbon dioxide, water and sulphur dioxide.
- Combustion is called incomplete if carbon monoxide appears in product gases, because carbon monoxide further react with oxygen to give  $\text{CO}_2$ .
- To provide energy to process industries various fuels are burnt with oxygen.
- Fuels can be divided into
  - (i.) Solids fuels
  - (ii.) Liquid fuels
  - (iii.) Gaseous fuels
- Example of solid fuels is coke, wood, coal, lignite etc.
- Example of liquid fuels is gasoline, kerosine, diesel fuel, fuel oil, biodiesel etc.
- Example of gaseous fuels are natural gas, producer gas, LPG (liquefied petroleum gas) etc.

### Combustion Reaction:

A combustion reaction is a major class of chemical reactions. Combustion usually occurs when a hydrocarbon reacts with water to produce carbon dioxide and water. In the more general sense, combustion involves a reaction between any combustible material and an oxidizer to form an oxidized product. Combustion is an exothermic reaction, so it releases heat, but sometimes the reaction proceeds so slowly that a temperature change is not noticeable.

### General Form of a Combustion Reaction

Hydrocarbon + Oxygen  $\rightarrow$  Carbon dioxide + Water

- (i)  $\text{C} + \text{O}_2 \rightarrow \text{CO}_2$  (Exothermic)
- (ii)  $\text{C} + 1/2 \text{O}_2 \rightarrow \text{CO}$  (Exothermic)
- (iii)  $\text{CO} + 1/2 \text{O}_2 \rightarrow \text{CO}_2$  (Exothermic)
- (iv)  $\text{C} + \text{CO}_2 \rightarrow 2 \text{CO}$  (Exothermic)
- (v)  $\text{H}_2 + 1/2 \text{O}_2 \rightarrow \text{H}_2\text{O}$  (Exothermic)
- (vi)  $\text{S} + \text{O}_2 \rightarrow \text{SO}_2$  (Exothermic)
- (vii)  $\text{CH}_4 + 2 \text{O}_2 \rightarrow \text{CO}_2 + 2 \text{H}_2\text{O}$  (Exothermic)

*Note: All combustion reactions are exothermic.*

### Types of Combustion:

**Complete Combustion:** Complete (clean) combustion with a hydrocarbon produces carbon dioxide and water.

**Incomplete Combustion:** Incomplete (dirty) combustion with a hydrocarbon produces carbon and/or carbon monoxide as well as carbon dioxide and water.





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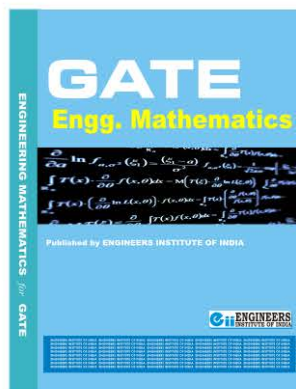
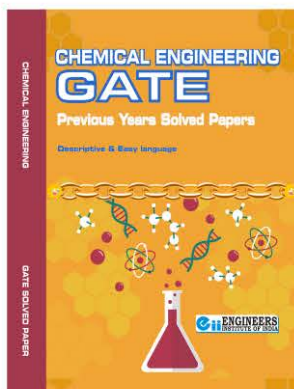
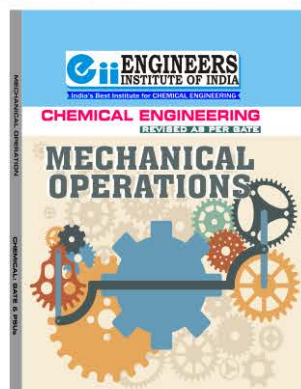
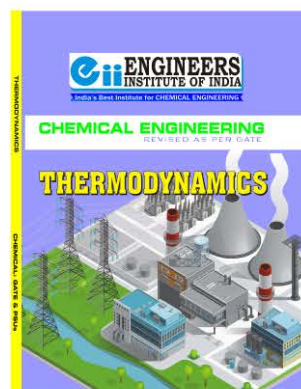
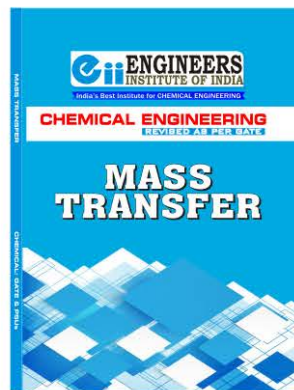
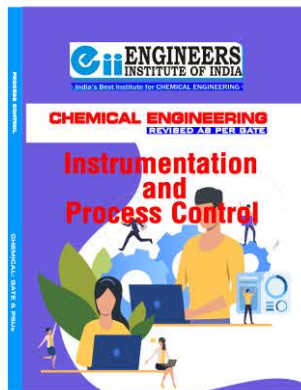
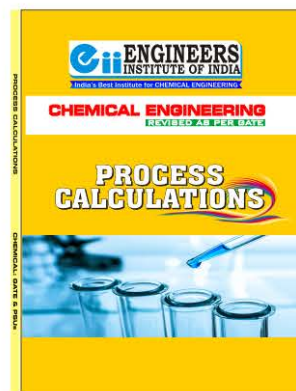
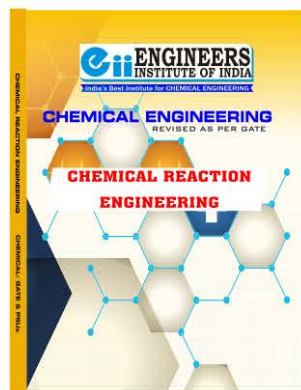
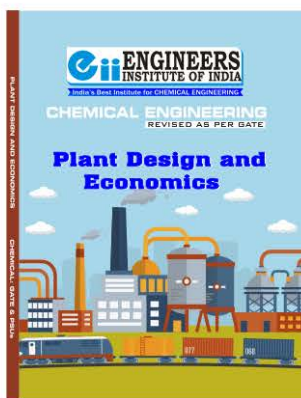
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