CHEMICAL ENGINEERING

Process Calculations

Comprehensive Theory
with Solved Examples *and* Practice Questions

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Process Calculations

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Process Calculations

CHAPTER

1

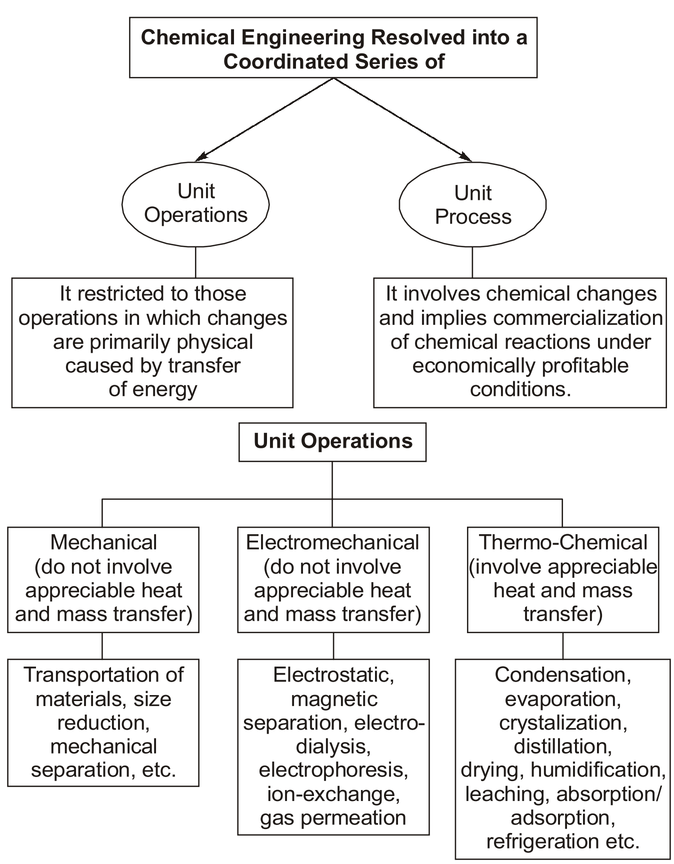
Introduction and Basic Concepts

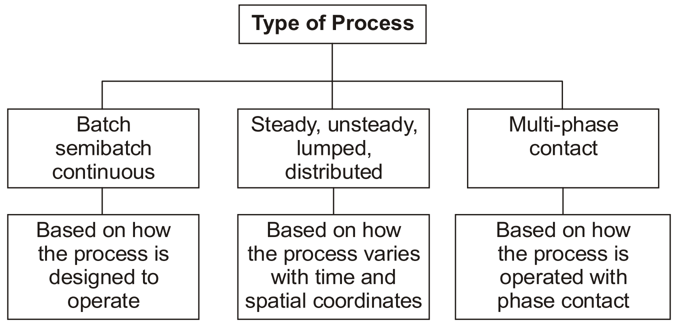
LEARNING OBJECTIVES

The reading of this chapter will enable the students

- To understand unit and dimensions.
- To understand the basic chemical calculations.
- To understand about ideal gas law and their applications.
- To understand about Raoult's and Henry's law for gas-liquid system.

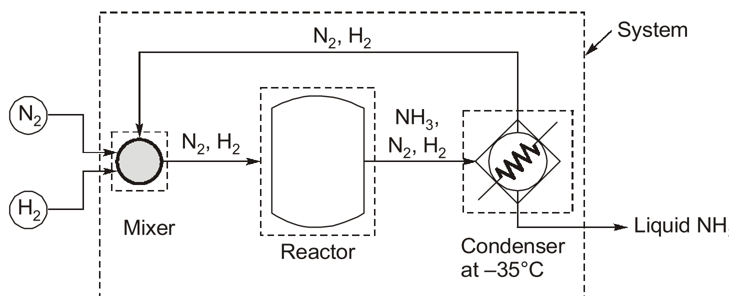
1.1 Introduction





What is System?

- Any specified arbitrary portion or whole of a process analyzing the problem is defined as system.
- It depends on what information is provided and what needs to be determined.
- A system may contain more than one process unit.
- In figure, the entire process is a system which consists of three process units.



1.2 Unit and Dimensions

Unit	Dimensions
• The "unit" indicates what the measured quantity represents.	• The "dimension" is the measurable quantity that the unit represents. Example : length, mass, time and temperature
• A measured or counted quantity has a numerical value and a unit.	• It also be calculated by multiplying or dividing other dimensions. Example : length/time = velocity, length^3 = volume and mass/length^3 = density
• Measurable units are specific values of dimensions that have been defined by convention. Example: grams for mass, seconds for time and centimeters for length	

The system of units composed of (1) Base units, (2) Derived units and (3) Multiple units.

1. **Base units:** These are the units for basic quantities such as length, mass, time, etc.
2. **Derived units:** These are the units obtained by multiplying and dividing base units. e.g., cm^2, m/s, etc.

3. **Multiple units:** These are the units which are multiple or fractions of base units. e.g., hour, minute, second, etc.

Unit Systems

The various systems of units and the basic/fundamental quantities associated with them are given below:

Fundamental Quantity	Systems of Units				Dimensions
	SI	MKS	CGS	FPS	
Length	Meter (m)	Meter (m)	Centimeter (cm)	Foot (ft)	L
Mass	Kilogram (kg)	Kilogram (kg)	Gram (g)	Pound (lb)	M
Time	Second (s)	Second (s)	Second (s)	Second (s)	θ
Temperature	Kelvin (K)	Celsius (°C)	Celsius (°C)	Fahreinheit (°F)	T

°C = Degrees Celsius
K = Kelvin
SI = International system of units

Symbolic abbreviations of the units are given in brackets.

(i) **Force:** According to Newton's law of motion, force is proportional to the product of mass and acceleration.

$$F \propto m.a$$
$$F = k\,m.a$$

In CGS system, dyne is defined as the force necessary to accelerate one gram mass at 1 cm/s^2.
In the SI system, Newton (N) is defined as the force necessary to accelerate one kilogram mass at 1 m/s^2. The engineer's unit of force in the MKS system is kilogram-force (kgf). The kilogram force is the force necessary to accelerate 1 kg mass at 9.81 m/s^2.
In the SI system, the unit of force has been named as Newton (N) in honour of the scientist Newton. 1 N is equal to 1 (kg.m)/s^2.

(ii) **Kilogram force (kgf):** The **kilogram force** is a metric unit of force (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^2. Then one (1) kilogram-force is equal to 1 kg × 9.80665 meter per second^2 = 9.80665 kilogram × meter per second^2 = 9.80665 newton (1 N).
Note: A kilogram-force (kgf), also called kilopond (kp), is a gravitational metric unit of force.

(iii) **Pressure:** Pressure is defined as the force per unit area.

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

The units of pressure in SI, MKS and FPS systems are N/m^2 (known as Pascal, abbreviated as Pa), kgf/cm^2 and lbf/in^2 (psi) respectively. The relationship between the absolute, atmospheric and gauge pressure is

Absolute pressure = Gauge pressure + Atmospheric pressure

Gauge pressure:

SI unit = N/m^2 (or Pa)

$$\text{CGS unit} = \text{dyn/cm}^2$$
$$\text{AES unit} = \text{lbf/in}^2 \text{ (or psi)}$$

- The gauge pressure of the fluid which is the pressure of the fluid relative to atmospheric pressure (refrence presure).
- A gauge pressure of 0 indicates that the absolute pressure of the fluid is equal to the atmospheric pressure.

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

Types of Pressures

- **Atmospheric pressure:** P_{atm}, is the pressure caused by the weight of the earth's atmosphere. Often atmospheric pressure is called barometric pressure.
- **Absolute pressure:** P_{abs}, is the total pressure. An absolute pressure of 0.0 is a perfect vacuum. Absolute pressure must be used in all calculations, unless a pressure difference is used.
- **Gauge pressure:** P_{gauge}, is pressure relative to atmospheric pressure.
- **Vacuum pressure:** P_{vacuum}, is a gauge pressure that is below atmospheric pressure.

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

(iv) **Work:** Work is defined as the product of the force acting on body and the distance travelled by the body in the direction of force applied.
The SI units for work are the joule (J) or Newton meter ($N \times m$), from the function $W = F \times s$ where W is work, F is force, and s is the displacement. The joule is also the SI unit of energy.

$$\text{Joule} = \text{N.m} = \text{kg.m}^2/\text{s}^2$$

(v) **Power:** Power is the time rate at which work is done or energy is transferred. In calculus terms, power is the derivative of work with respect to time.
The SI unitof power is the watt (W) or joule per second (J/s). Horsepower is a unit of power in the British system of measurement.

$$\text{Power} = \frac{\text{Work}}{\text{Time}}$$

or

$$P = \frac{W}{t}$$

(vi) **Heat:** It is a form of energy that flows from one body to another as a result of a difference in temperature. It cannot be stored as such within the system. The units of heat in SI, MKS and CGS systems are Joule (J), kilocalorie (kcal) and calorie (cal) respectively.

Example 1.1 **In a multiple effect evaporator system, the second effect is maintained under vacuum of 475 torr (mm Hg). Find the absolute pressure in kPa.**

Solution :

$$\text{Absolute pressure} = \text{Atmospheric pressure} - \text{Vacuum}$$
$$= 760 - 475 = 285 \text{ torr (mm Hg)}$$
$$\text{Absolute pressure} = 285 \text{ mm Hg} \times \left(\frac{101.325 \text{ kPa}}{760 \text{ mm Hg}}\right) = 38 \text{ kPa}$$

Example 1.2 A force of 19.635 kgf is applied on a piston of diameter 5 cm. Find the pressure exerted on the piston in kPa.

Solution :

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

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

$$F = 19.635 \text{ kgf}$$

$$P = \frac{19.635}{19.635} = 1 \text{ kgf/cm}^2$$

$$P = 1 \text{ kgf/cm}^2 \times \frac{101.325 \text{ kPa}}{1.033227 \text{ kgf/cm}^2} = 98.066 \text{ kPa}$$

Example 1.3 Consider the equations $S = 7t + 8t^2$, where $S = m$ and $t = s$. What are the dimensions and units of 7 and 8?

Solution :
Unit of 7 is m/s and 8 is m/s^2.

Example 1.4 The thermal conductivity k of a liquid metal is predicted via the empirical equation $k = A \exp(B/T)$, where k is in J/(s.m.K) and A and B are constants, T is absolute temperature. What are the units of A and B?

Solution :
A has the same unit as k i.e., J/(s.m.K), B has the unit of T i.e., K.

1.3 Basic Chemical Calculations

(i) **Atomic weight:** The atomic weight of an element is the mass of the atom of this element based on the scale that assigns carbon a mass of exactly twelve.

(ii) **Molecular weight:** The molecular weight of a compound is the sum of the atomic weights of atoms that constitute a molecule of the compound.

The molecular weight of a monoatomic element (e.g., sodium) is its atomic weight and the molecular weight of a diatomic element (e.g., oxygen, chlorine) is twice that of its atomic weight.

(iii) **Gram atom:** It is used to specify the amounts of chemical elements. It is defined as the mass in grams of an element which is numerically equal to its atomic weight.

$$\text{Gram atoms of an element} = \frac{\text{Weight in grams}}{\text{Atomic weight}} \quad \text{...(1.1)}$$

$$\therefore \quad \text{Gram atoms of element } A = \frac{\text{Weight in grams of } A}{\text{Atomic weight of } A} \quad \text{...(1.2)}$$

Similarly, the mass in kilograms of a given element that is numerically equal to its atomic weight is called a kilogram-atom.

Similarly, kilogram atoms of element $A = \dfrac{\text{Weight in kilograms of } A}{\text{Atomic weight of } A}$ ...(1.3)

For chemical compounds, a mole is defined as the amount of substance equal to its molecular weight/formula weight.

(iv) **Gram mole:** It is used to specify the amounts of chemical compounds. It is defined as the mass in grams of a substance that is equal numerically to its molecular weight.

$\therefore$ Gram moles of compound $B = \dfrac{\text{Weight in grams of } B}{\text{Molecular weight of } B}$ ...(1.4)

A gram mole of a substance is the mass in grams of the substance that is numerically equal to its molecular weight.

Similarly, Kg. moles of compound $B = \dfrac{\text{Weight in kilograms of } B}{\text{Molecular weight of } B}$ ...(1.5)

A mole is defined as the amount of a substance equal to its molecular weight.

Molecular weight of a compound is found from the atomic weight of elements involved in formation of the compound.

Example 1.5 Calculate the kilogram atoms of carbon which weighs 36 kg.

Solution :

$$\text{Atomic weight of carbon} = 12$$

$$\therefore \quad k\text{-atom of carbon} = \frac{\text{Weight in kilograms of carbon}}{\text{Atomic weight of carbon}} = \frac{36}{12} = 3$$

Example 1.6 Calculate the kilograms of Na of which the amount is specified as 3 k-atom.

Solution :

Basis: 3 k-atom Na.

$$\text{Atomic weight of Na} = 23$$

$$\therefore \quad \text{k-atom of Na} = \frac{\text{kg of Na}}{\text{Atomic weight of Na}}$$

$$\therefore \quad \text{kg of Na} = k\text{-atom of Na} \times \text{Atomic weight of Na}$$

$$= 3 \times 23 = 69$$

(v) **Equivalent weight of an element or a compound** is defined as the ratio of the atomic weight or molecular weight to its valence. The valence of an element or a compound depends on the number of hydroxyl ions (OH^-) donated or the hydrogen ions (H^+) accepted for each atomic weight or molecular weight.

$\therefore$ Equivalent weight $= \dfrac{\text{Molecular weight}}{\text{Valence}}$ ...(1.6)

The concentration of a solution containing a solid or a liquid solute can be expressed in terms of normality, molarity and molality.

(vi) **Normality** is designated by the symbol N and is defined as the number of gram-equivalent of solute dissolved in one litre of solution [for preparation of 1 N NaOH solution, we have to dissolve 40 grams of NaOH ($\equiv$ to 1 g equivalent of NaOH) in one litre of solution (solvent-water)].

$$\text{Normality (N)} = \frac{\text{gram-equivalents of solute}}{\text{Volume of solution in litre}} \quad ...(1.7)$$

(vii) **Molarity:** It is defined as the number of gram moles of solute dissolved in one litre of solution. It is designated by the symbol M.

$$\text{Molarity (M)} = \frac{\text{gram moles of solute}}{\text{Volume of solution in litre}}$$

(viii) **Molality:** It is defined as the number of gram-moles (mol) of solute dissolved in one kilogram of solvent.

$$\text{Molality} = \frac{\text{gram moles of solute}}{\text{Mass of solvent in kg}} \quad ...(1.8)$$

From the definition of normality, thus, it is possible to find the concentration of solute in *g/l*.

$$\text{Concentration } (g/l) = \text{Normality} \times \text{Equivalent weight} \quad ...(1.9)$$

Example 1.7 Find the equivalent weights of (1) HCl, (2) NaOH, (3) Na_2CO_3 and (4) H_2SO_4.

Solution :

1. HCl

$$\text{Molecular weight of HCl} = 1 \times 1 + 1 \times 35.5 = 36.5$$
$$\text{Valence of HCl} = 1$$
$$\therefore \quad \text{Equivalent weight of HCl} = \frac{36.5}{1} = 36.5$$

2. NaOH

$$\text{Molecular weight of NaOH} = 1 \times 23 + 1 \times 16 + 1 \times 1 = 40$$
$$\text{Valence of NaOH} = 1$$
$$\therefore \quad \text{Equivalent weight of NaOH} = \frac{40}{1} = 40$$

3. Na_2CO_3

$$\text{Molecular weight of } Na_2CO_3 = 2 \times 23 + 1 \times 12 + 3 \times 16 = 106$$
$$\text{Valence of } Na_2CO_3 = 2$$
$$\therefore \quad \text{Equivalent weight of } Na_2CO_3 = \frac{106}{2} = 53$$

4. H_2SO_4

$$\text{Molecular weight of } H_2SO_4 = 2 \times 1 + 1 \times 32 + 4 \times 16 = 98$$
$$\text{Valence of } H_2SO_4 = 2$$
$$\therefore \quad \text{Equivalent weight of } H_2SO_4 = \frac{98}{2} = 49$$

Example 1.8 20 g of caustic soda is dissolved in water to prepare 500 ml of solution. Find the normality and molarity of solution?

Solution :

Basis: 500 ml of solution.

$$\text{Amount of caustic soda dissolved} = 20 \text{ g}$$

$$\text{Molecular weight of NaOH} = 40$$

$$\text{Equivalent weight of NaOH} = \frac{40}{1} = 40$$

$$\text{Volume of solution} = 500 \text{ ml} = 0.5 l$$

$$\text{Gram-equivalents of NaOH} = \frac{20}{40} = 0.5 \text{ g.eq}$$

$$\therefore \quad \text{Normality (N)} = \frac{\text{g-eq of NaOH}}{\text{Volume of solution in } l} = \frac{0.5}{0.5} = 1$$

$$\text{Moles of NaOH} = \frac{20}{40} = 0.5 \text{ mol}$$

$$\therefore \quad \text{Molarity (M)} = \frac{\text{Moles of NaOH}}{\text{Volume of solution in } l} = \frac{0.5}{0.5} = 1$$

Example 1.9 A chemist is interested in preparing 500 ml of 1 normal, 1 molar and 1 molal solutionof H_2SO_4. Assuming the density of H_2SO_4 solution to be 1.075 g/cm^3, calculate the quantities of H_2SO_4 to be taken to prepare these solutions.

Solution :

Basis: 500 ml of H_2SO_4 solution.

$$\text{Volume of solution} = 500 \text{ m}l = 0.5 \ l$$

$$\text{Normality} = \frac{\text{gram-equivalents of } H_2SO_4}{\text{Volume of solution in litre}}$$

$$\therefore \quad \text{gram-equivalents of } H_2SO_4 = \text{Normality} \times \text{Volume of solution}$$

$$= 1 \times 0.5 = 0.5 \text{ g eq}$$

$$\text{Molecular weight of } H_2SO_4 = 98$$

$$\therefore \quad \text{Equivalent weight of } H_2SO_4 = \frac{98}{2} = 49$$

Amount of H_2SO_4 required for 1 normal solution

$$= 0.5 \times 49 = 24.5 \text{ g}$$

$$\text{Molarity} = \frac{\text{gram moles of } H_2SO_4}{\text{Volume of solution in litre}}$$

$$\text{Moles of } H_2SO_4 = \text{Molarity} \times \text{Volume of solution} = 1 \times 0.5 = 0.5 \text{ mol}$$

$\therefore$ Amount of H_2SO_4 required to make 1 molar solution = $0.5 \times 98 = 49$ g

Let x be the quantity in grams of H_2SO_4 required for making 1 molal solution.

$$\text{Density of solution} = 1.075 \text{ g/cm}^3$$

$$\text{Quantity of solution} = 500 \times 1.075 = 537.5 \text{ g}$$

$$\text{Grams of solvent} = \text{Grams of solution} - \text{Grams of solute} = 537.5 - x$$

$$\text{Weight of solvent} = (537.5 - x) \times 10^{-3} \text{ kg}$$

$$\text{Molecular weight of } H_2SO_4 = 98$$

$$\text{Moles of } H_2SO_4 = \frac{x}{98} \text{ mol}$$

$$\text{Molality} = \frac{\text{gram moles of solute}}{\text{Weight of solvent in kg}}$$

Example 1.19 Carbon dioxide weighing 1.10 kg occupies a volume of 33 litres at 300 K. Calculate the pressure using the Van der Waals equation of state.

Data: $a = 3.60\ (m^3)^2$, $kPa/(kmol)^2$ and $b = 4.3 \times 10^{-2}\ m^3/kmol$ for CO_2

Solution :

Basis: 1.10 kg of CO_2 gas at 300 K.

The Van der Waals equation is

$$\left(P + \frac{a}{V^2}\right)(V - b) = RT$$

$$\text{Amount of } CO_2 \text{ gas} = 1.10 \text{ kg} = 0.025 \text{ kmol}$$

$$\text{Volume occupied by this gas} = 33l = 0.033\ m^3$$

$$\therefore \quad V = \frac{0.033}{0.025} = 1.32\ m^3/kmol$$

$$a = 3.60\ (m^3)^2\ kPa/(kmol)^2$$

$$b = 4.3 \times 10^{-2}\ m^3/kmol$$

$$R = 8.31451\ (m^3.kPa)/(kmol.K)$$

$$T = 300\ K$$

$$\left[P + \frac{3.60}{(1.32)^2}\right][1.32 - 4.3 \times 10^{-2}] = 8.31451 \times 300$$

Solving we get, $P = 1951\ kPa = 1.951\ MPa$

Compressibility factor: Compressibility factor (Z) is defined as

$$Z = \frac{PV}{nRT}$$

$$Z = \frac{\text{Actual volume of gas at a given temperture and pressure}}{\text{Volume of the ideal gas at the same } T \text{ and } P}$$

Student's Assignments

Q.1 Convert a pressure of 2 atm to mm Hg.

Q.2 Convert a volumetric flow rate of 2 m^3/s to l/s.

Q.3 Convert 88 kg of carbon dioxide into its amount in molar units.

Q.4 Find the moles of oxygen present in 500 grams.

Q.5 Find moles of K_2CO_3 that will contain 117 kg of K.

Q.6 How many kilograms of carbon are present in 64 kg of methane?

Q.7 98 grams of sulphuric acid (H_2SO_4) are dissolved in water to prepare one litre of solution. Find normality and molarity of solution.

Q.8 A solution of caustic soda contains 20% NaOH by weight. Taking density of the solution as 1.196 kg/l, find the normality, molarity and molality of the solution.

Q.9 H_2SO_4 solution has a molarity of 11.24 and molality of 94. Calculate the density of solution.

Q.10 At 298 K (25°C) the solubility of methyl bromide in methanol is 44 kg per 100 kg. Calculate : (i) the weight fraction and (ii) the mole fraction of methanol in the saturated solution.

Q.11 Calculate the weight of sulphur dioxide in a vessel having 2 m^3 volume, the pressure and temperature being 97.33 kPa and 393 K (120°C).

Q.12 A certain quantity of gas contained in a closed vessel of volume 1 m^3 at a temperature of 298 K (25°C) and pressure of 131.7 kPa is to be heated such that the pressure should not exceed 303.98 kPa. Calculate the temperature of gas attained.

Q.13 A mixture of nitrogen and carbon dioxide at 298 K (25°C) and 101.325 has an average molecular weight of 31. What is the partial pressure of nitrogen?

Q.14 960 cc of a gas weighs 2.5 g at 750 torr and 300 K (27°C). Calculate the molecular weight of gas.

Q.15 A sample of gas having volume of 10 *l* at 101.325 kPa pressure and at temperture of 298 K (25°C) is compressed to a high pressure so that its volume reduces by 4.5 *l*. If the pressure rises by 0.1 MPa, what will be the rise in temperature?

ANSWERS

1. (1520)	**2.** (2000)	**3.** (2)	**4.** (15.625)
5. (1.5)	**6.** (48)	**7.** (2, 1)	
8. (5.98, 5.98, 6.25)		**9.** (1.2205)	
10. (0.6944, 0.871)		**11.** (3.8144)	**12.** (687.82)
13. (82.33)	**14.** (65)	**15.** (27.6)	

Explanation

1. (1520)

Basis : 2 atm pressure.

Conversion factor between atm and mm Hg is 1 atm = 760 mm Hg.

$\therefore \quad 2 \text{ atm} = ?$

$$\therefore \quad \text{Pressure} = 2 \text{ atm} \times \left(\frac{760 \text{ mm Hg}}{1 \text{ atm}}\right) = 1520 \text{ mm Hg}$$

2. (2000)

Basis : Volumetric flow rate of 2 m^3/s.

Relationship between volume in m^3 and volume in *l* is

$$1 \text{ m}^3 = 1000\, l$$

$\therefore$ Volumetric flow rate

$$= 2 \text{ m}^3/\text{s} \times \frac{1000\, l}{1 \text{ m}^3} = 2000\, l/\text{s}$$

3. (2)

Basis : 88 kg of carbon dioxide.

Molecular formula of carbon dioxide = CO_2

Atomic weight: C = 12 and O = 16

Molecular weight of $CO_2 = 1 \times 12 + 2 \times 16 = 44$

$$\text{kmol of } CO_2 = \frac{\text{kg of } CO_2}{\text{Molecular weight of } CO_2} = \frac{88}{44} = 2$$

$\therefore$ 88 kg of CO_2 = 2 kmol CO_2

4. (15.625)

Basis : 500 g of oxygen.

Molecular weight of $O_2 = 2 \times 16 = 32$

$$\text{Moles of } O_2 = \frac{500}{32} = 15.625 \text{ mol}$$

5. (1.5)

Basis : 117 kg of K.

Atomic weight of K = 39

$$\text{Atoms of K} = \frac{117}{39} = 3 \text{ katom}$$

Each mole of K_2CO_3 contains 2 atom of K

2 atom of K $\equiv$ 1 mole of K_2CO_3

2 katom of K $\equiv$ 1 kmol of K_2CO_3

$$\therefore \text{ Moles of } K_2CO_3 = \frac{1}{2} \times 3 = 1.5 \text{ kmol}$$

6. (48)

Basis : 64 kg of methane.

Atomic weight of C = 12

Molecular weight of CH_4 = 16

1 katom of carbon $\equiv$ 1 kmol of CH_4

$\therefore$ 12 kg of carbon $\equiv$ 16 kg of CH_4

i.e., in 16 kg of CH_4, 12 kg of carbon are present.

So, amount of carbon present in 64 kg of methane

$$= \frac{12}{16} \times 64 = 48 \text{ kg}$$