CHAPTER 2: MOLES, DENSITY, AND CONCENTRATION

2.1 The Mole

- **mole** is a certain amount of material corresponding to a specified number of molecules, atoms, electrons, or any other specified types of particles.

- In SI system a mole is the amount of a substance that contains as many elementary entities (6.022×10^{23})as there are atoms in 0.012 kg of carbon 12, or there are 6.022×10^{23} atoms of carbon in 12 grams of carbon-12

- To keep the units straight we will use the gmole for the SI mole . The **pound mole** (Ib mol, comprised of $6.022 \times 10^{23} \times 453.6$) molecules, the kg mol (kilomole, kmol, comprised of 1,000 moles), and so on.

MOLES, DENSITY, AND CONCENTRATION

$$\text{molecular weight (MW)} = \frac{\text{mass}}{\text{moles}}$$

$$\text{the g mol} = \frac{\text{mass in g}}{\text{molecular weight}}$$

$$\text{the lb mol} = \frac{\text{mass in lb}}{\text{Molecular weight}}$$

Example:

$$\frac{100.0 \text{ g } H_2O}{} \left| \frac{1 \text{ g mol } H_2O}{18.0 \text{ g } H_2O} \right. = 5.56 \text{ g mol } H_2O$$

$$\frac{6.0 \text{ lb mol } O_2}{} \left| \frac{32.0 \text{ lb } O_2}{1 \text{ lb mol } O_2} \right. = 192 \text{ lb } O_2$$

- the **atomic weight** of an element is the mass of an atom based on the scale that assigns a mass of exactly 12 to the carbon isotope.

- the **molecular weight** of the compound is nothing more than the sum of the weights of atoms of which it is composed

Example: Use the Molecular Weights to Convert Mass to Moles If a bucket holds 2.00 lb of NaOH, how many:

(a) Pound moles of NaOH does it contain?

(b) Gram moles of NaOH does it contain?

Solution:

$$\text{(a)}\quad \frac{2.00\ \text{lb NaOH}}{} \left| \frac{\mathbf{1\ lb\ mol\ NaOH}}{40.0\ \text{lb NaOH}} \right. = 0.050\ \text{lb mol NaOH}$$

$$\text{(b}_1\text{)}\quad \frac{2.00\ \text{lb NaOH}}{} \left| \frac{\mathbf{1\ lb\ mol\ NaOH}}{40.0\ \text{lb NaOH}} \right| \frac{454\ \text{g mol}}{1\ \text{lb mol}} = 22.7\ \text{g mol}$$

Example: How many pounds of NaOH are in 7.50 g mol of NaOH?

Solution:

Basis: 7.50 g mol of NaOH

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

2.2 Density

➢ **Density** is the ratio of mass per unit volume, as for example, kg/m^3 or lb/ft^3.

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

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

Example: the density of n-propyl alcohol is 0.804 g/cm^3, what would be the volume of 90.0 g of the alcohol?

Solution:

$$\frac{90.0\ g}{} \left| \frac{1\ cm^3}{0.804\ g} \right. = 112\ cm^3$$

- molar density **(ρ/MW)**

  molar volume **(MW/ρ)**

- For some solutions, to calculate the density of the solution, you can make a linear combination of the individual components by adding the respective masses and volumes, and then dividing:

$$V = \sum_{i=1}^{n} V_i \qquad \text{where } n = \text{number of components}$$

$$m = \sum_{i=1}^{n} m_i$$

$$\rho_{\text{solution}} = \frac{m}{V}$$

2.3 Specific Gravity

- Specific gravity is a dimensionless ratio. Actually, it should be considered as the ratio of two densities-that of the substance of interest, A, to that of a reference substance.

$$\text{sp.gr. of } A = \textbf{specific gravity} \text{ of } A = \frac{(\text{g/cm}^3)_A}{(\text{g/cm}^3)_{ref}} = \frac{(\text{kg/m}^3)_A}{(\text{kg/m}^3)_{ref}} = \frac{(\text{lb/ft}^3)_A}{(\text{lb/ft}^3)_{ref}}$$

- The reference substance for liquids and solids normally is water which has a density of 1.000 g/cm^3, 1000 kg/m^3, or 62.43 lb/ft^3 at 4^{O}C.

- The specific gravity of gases frequently is referred to air, but may be referred to other gases.

Example: If a 70% (by weight) solution of glycerol has a specific gravity of 1.184 at 15°C, what is the density of the solution in:

(a) g/cm3? (b) lb_m/ft^3? and (c) kg/m^3?

Solution: assume that the temperatures of the water is 4°C, and that water has a density of 1 .00 x $l0^3$ kg/m^3 (1 .00 g/cm^3).

(a) 1.184 g solution/cm^3

(b) (1.184 lb glycerol/ft^3)/(1 Ib water/ft^3) x (62.4 Ib water/ft^3) = 73.9 lb solution/ ft^3

(c) 1.184 x $l0^3$ kg solution/m^3.

- In the petroleum industry the specific gravity of petroleum products is often reported in terms of a hydrometer scale called °API. The equation for the API scale is:

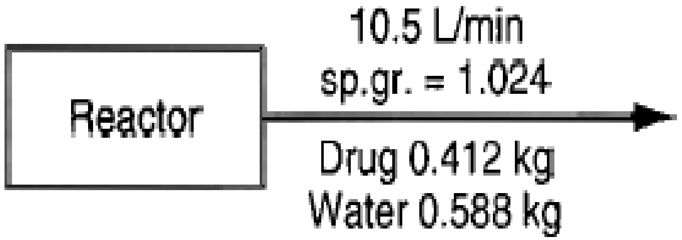
$$°\text{API} = \frac{141.5}{\text{sp.gr.}\frac{60°\text{F}}{60°\text{F}}} - 131.5 \qquad (\text{API gravity})$$

$$\text{sp.gr.}\frac{60°}{60°} = \frac{141.5}{°\text{API} + 131.5}$$

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

Solution:

Basis: 1.000 kg solution



$$\text{density of solution} = \frac{1.024\,\frac{\text{g soln}}{\text{cm}^3}}{1.000\,\frac{\text{g H}_2\text{O}}{\text{cm}^3}} \left| \frac{1.000\,\frac{\text{g H}_2\text{O}}{\text{cm}^3}}{} \right. = 1.024\,\frac{\text{g soln}}{\text{cm}^3}$$

Next convert the amount of drugs of solution to mass per volume

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

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

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

2.4 Flow Rate

- the **flow rate** of a process stream is the rate at which material is transported through a pipe

Mass flow rate = $\dot{m} = \frac{m}{t}$

Volumetric flow rate = $F = \frac{V}{t}$

Molar flow rate = $\dot{n} = \frac{n}{t}$

2.5 Mole Fraction and Mass (Weight) Fraction

- **Mole fraction** is the number of moles of a particular compound in a mixture or solution divided by the total number of moles in the mixture or solution.

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

- the **mass (weight) fraction** is the **mass (weight)** of the compound divided by the total mass (weight) of all of the compounds in the mixture or solution.

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

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

Solution:

Basis: 10.0 kg of total solution

Component	kg	Weight fraction	Mol. Wt.	kg mol	Mole fraction
H_2O	5.00	$\frac{5.00}{10.0} = 0.500$	18.0	0.278	$\frac{0.278}{0.403} = 0.69$
NaOH	5.00	$\frac{5.00}{10.00} = 0.500$	40.0	0.125	$\frac{0.125}{0.403} = 0.31$
Total	10.00	1.000		0.403	1.00

The kilogram moles are calculated as follows:

$$\frac{5.00 \text{ kg } H_2O}{} \left| \frac{1 \text{ kg mol } H_2O}{18.0 \text{ kg } H_2O} \right. = 0.278 \text{ kg mol } H_2O$$

$$\frac{5.00 \text{ kg NaOH}}{} \left| \frac{1 \text{ kg mol NaOH}}{40.0 \text{ kg NaOH}} \right. = 0.125 \text{ kg mol NaOH}$$

Adding these quantities together gives the total kilogram moles.

2.6 Analyses of Multi-component Solutions and Mixtures

- The composition of gases will always be presumed to be given in mole percent or fraction unless specifically stated otherwise.

- The composition of liquids and solids will be given by mass (weight) percent or fraction unless otherwise specifically stated, as is the common practice in industry.

Example: what is the molecular weight of air based on the assumption that all of the air that is not O_2 is N_2 with a pseudo-molecular weight of 28.2.

Solution:

Component	Moles = percent	Mol. wt.	Lb or kg	Weight %
O_2	21.0	32	672	23.17
N_2	79.0	28.2	2228	76.83
Total	100		2900	100.00

The average molecular weight is 2900 lb/100 lb mol = 29.0, or 2900 kg/100 kg mol = 29

2.7 Concentration

- **Concentration** generally refers to the quantity of some substance per unit volume
- Mass per unit volume (lb of solute/ft3 of solution, g of solute/L, lb of solute/barrel, kg of solute/m^3).
- Moles per unit volume (lb mol of solute/ft^3 of solution, g mol of solute/L, g mol of solute/cm^3).
- Parts per million **(ppm);** parts per billion (ppb), a method of expressing the concentration of extremely dilute solutions.

- Parts per million by volume (ppmv) and parts per billion by volume (ppbv)

- Other methods of expressing concentration are molarity (g mol/L), molality (mole solute/kg solvent), and normality (equivalents/L).

Example: A solution of HNO_3 in water has a specific gravity of 1.10 at 25°C. The concentration of the HNO_3 is 15 g/L of solution. What is the

a. Mole fraction of HNO_3 in the solution?

b. Ppm of HNO_3 in the solution?

Solution:

Basis: 1 L of solution

$$\frac{15 \text{ g } HNO_3}{1 \text{ L soln}} \left| \frac{1 \text{ L}}{1000 \text{ cm}^3} \right| \frac{1 \text{ cm}^3}{1.10 \text{ g soln}} = 0.01364 \frac{\text{g } HNO_3}{\text{g soln}}$$

Basis: 100 g solution

The mass of water in the solution is: 100 − 0.0134 = 99.986 g H_2O.

		g	MW	g mol	mol fraction
a.	HNO_3	0.01364	63.02	2.164×10^{-4}	3.90×10^{-5}
	H_2O	99.986	18.016	5.550	1.00
	Total			5.550	1.00

b. $$\frac{0.01364}{1} = \frac{13{,}640}{10^6} \text{ or } 13{,}640 \text{ ppm}$$