Lecture 4

Moles, Density and Concentration

The mole

<u>The atomic weight</u> of an element is the mass of an atom based on the scale that assigns a mass of exactly 12 to the carbon isotope ^{12}C.

A <u>compound</u> is composed of more than one atom, and the molecular weight of the compound is nothing more than the sum of the weights of atoms of which it is composed**.**

In the SI system, a **<u>mole</u>** is composed of 6.022 x 10^{23} (Avogadro's number) molecules. To convert the number of moles to mass and the mass to moles, we make use of the molecular weight– the mass per mole:

$$\text{Molecular Weight} = \frac{\text{Mass}}{\text{Mole}}$$

Thus, the calculations you carry out are**:**

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

$$\text{The lb mol} = \frac{\text{mass in lb}}{\text{molecular weight}}$$

Example 9

How many of each of the following are contained in 100 g of CO_2 (M = 44.01)?

1. mol CO_2

$$\frac{100.0 \text{ g } CO_2}{} \left| \frac{1 \text{ mol } CO_2}{44.01 \text{ g } CO_2} \right. = \boxed{2.273 \text{ mol } CO_2}$$

2. lb moles CO_2

$$\frac{2.273 \text{ mol } CO_2 \;|\; 1 \text{ lb-mol}}{|\; 453.6 \text{ mol}} = \boxed{5.011 \times 10^{-3} \text{ lb-mole } CO_2}$$

3. mol C

$$\frac{2.273 \text{ mol } CO_2 \;|\; 1 \text{ mol C}}{|\; 1 \text{ mol } CO_2} = \boxed{2.273 \text{ mol C}}$$

4. mol O

$$\frac{2.273 \text{ mol } CO_2 \;|\; 2 \text{ mol O}}{|\; 1 \text{ mol } CO_2} = \boxed{4.546 \text{ mol O}}$$

5. mol O_2

$$\frac{2.273 \text{ mol } CO_2 \;|\; 1 \text{ mol } O_2}{|\; 1 \text{ mol } CO_2} = \boxed{2.273 \text{ mol } O_2}$$

6. g O

$$\frac{4.546 \text{ mol O} \;|\; 16.0 \text{ g O}}{|\; 1 \text{ mol O}} = \boxed{72.7 \text{ g O}}$$

7. g O_2

$$\frac{2.273 \text{ mol } O_2 \;|\; 32.0 \text{ g } O_2}{|\; 1 \text{ mol } O_2} = \boxed{72.7 \text{ g } O_2}$$

8. molecules of CO_2

$$\frac{2.273 \text{ mol } CO_2 \;|\; 6.02 \times 10^{23} \text{ molecules}}{|\; 1 \text{ mol}} = \boxed{1.37 \times 10^{24} \text{ molecules}}$$

9. kmol of CO_2 for 100 kg CO_2

$$\frac{100 \text{ kg } CO_2 \;|\; 1 \text{ kmol } CO_2}{|\; 44.0 \text{ kg } CO_2} = 2.27 \;\frac{\text{kmol } CO_2}{}$$

Example 10

Calculate the average molecular weight of air, assuming that air is 21% O_2 and 79% N_2.

Solution

Because the composition of air is given in mole percent, a basis of 1 g mol is chosen. The MW of the N_2 is not actually 28.0 but 28.2 because the value of the MW of the pseudo 79% N_2 is actually a combination of 78.084% N_2 and 0.934% Ar. The masses of the O_2 and pseudo N_2 are

Basis: 1 g mol of air

$$\text{Mass of } O_2 = \frac{1 \text{ g mol air}}{} \left| \frac{0.21 \text{ g mol } O_2}{\text{g mol air}} \right| \frac{32.00 \text{ g } O_2}{\text{g mol } O_2} = 6.72 \text{ g } O_2$$

$$\text{Mass of } N_2 = \frac{1 \text{ g mol air}}{} \left| \frac{0.79 \text{ g mol } N_2}{\text{g mol air}} \right| \frac{28.2 \text{ g } N_2}{\text{g mol } N_2} = 22.28 \text{ g } N_2$$

$$\text{Total} = 29.0 \text{ g air}$$

Therefore, the total mass of 1 g mol of air is equal to 29.0 g, which is called the average molecular weight of air. (Because we chose 1 g mol of air as the basis, the total mass calculated directly provides the average molecular weight of 29.0.)

Density

Density is the ratio of mass per unit volume, as for example, kg/m^3 or lb/ft^3. Density has both a numerical value and units. Specific volume is the inverse of density, such as cm^3/g or ft^3/lb.

$$\text{Density } (\rho) = \frac{\text{mass}}{\text{volume}} = \frac{m}{V}$$

$$\text{Specific volume}(\hat{V}) = \frac{\text{volume}}{\text{mass}} = \frac{V}{m}$$

For example, given that the density of n-propyl alcohol is 0.804 g/cm^3, what would be the volume of 90 g of the alcohol? The calculation is:

$$90 \text{ g} \left| \frac{1 \text{ cm}^3}{0.804 \text{ g}} \right. = 112 \text{ cm}^3$$

A homogeneous mixture of two or more components, whether solid, liquid, or gaseous, is called a solution.

For **some solutions**, the density of the solution is

$V = \sum_{i=1}^{n} V_i$

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

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

Where n is a number of components

Specific Gravity (SG)

The SG of a substance is the ratio of the density (ρ) of the substance to the density of a reference substance (ρ_{ref}) at a specific condition:

$$\text{SG of A} = \frac{\rho}{\rho_{ref}} = \frac{(g/cm^3)_A}{(g/cm^3)_{ref}} = \frac{(kg/m^3)_A}{(kg/m^3)_{ref}} = \frac{(lb/ft^3)_A}{(lb/ft^3)_{ref}}$$

♦ The reference substance for liquids and solids normally is water.

♦ The density of water is 1.000 g/cm^3, 1000 kg/m^3, or 62.43 lb/ft^3 at 4°C.

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

For Example If dibromopentane (DBP) has a specific gravity of 1.57, what is the density in (a) g/cm^3? (b) lb_m/ft^3? and (c) kg/m^3?

a) $\frac{1.57 \frac{g\ DBP}{cm^3}}{1 \frac{g\ H2O}{cm^3}} \Big| 1 \frac{g\ H2O}{cm^3} = 1.57 \frac{g\ DBP}{cm^3}$

b) $\frac{1.57 \frac{lb\ DBP}{ft^3}}{1 \frac{lb\ H2O}{ft^3}} \Big| 62.4 \frac{lb\ H2O}{ft^3} = 97.97 \frac{lb\ DBP}{ft^3}$

c) $1.57\ \frac{\text{g DBP}}{\text{cm}^3} \mid \left(\frac{100\text{ cm}}{1\text{ m}}\right)^3 \mid \frac{1\text{ kg}}{1000\text{ g}} = 1.57 * 10^3\ \frac{\text{kg DBP}}{\text{m}^3}$

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

$$ºAPI = \frac{141.5}{SG\ (at\ 60\ ºF)} - 131.5$$

Or,

$$\text{SG (at 60 ºF)} = \frac{141.5}{ºAPI + 131.5}$$

The volume and therefore the densityof petroleum products vary with temperature, and the petroleum industry has established 60 °F as the standard temperature for volume and API gravity.

Example 11

5,000 barrels of 28º API gas oil are blended with 20,000 bbl of 15º API fuel oil. What is the density of the mixture in lb/gal and lb/ft^3**?**Assume that the volumes are additive. Given that 1 bbl = 42 gal, 1 ft^3 = 7.48 gal and the density of water at 60 ºF is 0.999 g/cm^3.

Solution

$$\rho_{\text{mix}} = \frac{\text{lb of 28º oil+lb of 15º oil}}{\text{total volume}} = \frac{\text{lb of 28º oil+lb of 15º oil}}{\text{5000+20,000 bbl}}$$

$$\text{SG}_{(28º\text{ API})} = \frac{141.5}{28+131.5} = 0.887\ ; \quad \rho_{28º\text{ API}} = 0.887*62.4 = 55.36\ \text{lb}_m/\text{ft}^3$$

$$\text{SG}_{(15º\text{ API})} = \frac{141.5}{15+131.5} = 0.966\ ; \quad \rho_{15º\text{ API}} = 0.966*62.4 = 60.27\ \text{lb}_m/\text{ft}^3$$

$$\text{V}_{28º\text{ API}} = 5000\text{ bbl} \mid \frac{42\text{ gal}}{1\text{ bbl}} \mid \frac{1\text{ ft}^3}{7.481\text{ gal}} = 2.807 * 10^4\ \text{ft}^3$$

$$V_{15º\ API} = 20{,}000\ \text{bbl} \left| \frac{42\ \text{gal}}{1\ \text{bbl}} \right| \frac{1\ \text{ft}^3}{7.481\ \text{gal}} = 1.123 * 10^5\ \text{ft}^3$$

$$\rho_{mix} = \frac{\left(55.36\ \frac{\text{lb}_m}{\text{ft}^3}\right)*(2.807*10^4\ \text{ft}^3)+\left(60.27\ \frac{\text{lb}_m}{\text{ft}^3}\right)*\left(1.123*10^5\ \text{ft}^3\right)}{2.807*10^4\ +1.123*10^5\ \text{ft}^3} = 59.29\ \frac{\text{lb}_m}{\text{ft}^3}$$

$$= 7.93\,\frac{\text{lb}_m}{\text{gal}}$$