Lecture 3 -- Chapter 4 -- Equilibrium between Phases of Matter – Section 4.2

Learning Objectives:

1. Become familiar with different ways of expressing composition of mixtures.
2. Learn how to convert from one type of composition specification to another type.

In engineering sciences well as in everyday life, we encounter materials that are made up by mixing two or more components. A familiar example is a drink cocktail. You can describe such mixtures by saying things like it contains 1 part of component A, mixed with 3 parts of component B and 2 parts of component C. Such descriptions are not very useful for scientific purposes. It can become cumbersome to describe complex mixtures this way. Moreover, it is not obvious what is meant by the word "parts" in such a description. Does it weight or volume?

There are three accepted methods for specifying compositions.

- Mass fraction
- Mole fraction
- Volume fraction

<u>Mass-Fraction</u>

Mass fraction of Component i in a Mixture containing c components is denoted by W_i and is defined as

$$W_i = \frac{m_i}{m_1 + m_2 + m_3 + ----+ m_c}, \quad 1 \le i \le c \tag{4.1}$$

Where, m_i = mass of component i in the mixture and
c = number of components in the mixture

Note that the denominator is equal to the total mass of the mixture. So the mass fraction of component i tells you what fraction of the total mass of the mixture is composed of component i.

Example Problem 4-1

(a) A solution is made from 10 g of water and 30 g of pure ethyl alcohol. What is the mass fraction of alcohol?

(b) A gas mixture contains 21 kg of oxygen, 79 kg of nitrogen, and 900 kg of hydrogen sulfide. What are the mass fractions of the components?

Solution

(a) The total mass of the liquid solution is (10 + 30) or 40 g. The mass fraction of alcohol is

$$\frac{30 \text{ g alcohol}}{40 \text{ g solution}} = 0.75$$

(b)The total mass of the mixture is 1000 kg. The mass fractions of oxygen nitrogen and hydrogen sulfide are 0.021, 0.079 and 0.9 respectively. The sum of the mass fractions is l.0.

<u>Mole-Fraction</u>

Mole fraction of Component i in a Mixture containing c components is denoted by x_i and is defined as

$$x_i = \frac{n_i}{n_1 + n_2 + n_3 + - - - - + n_c}, \quad 1 \le i \le c \tag{4.2}$$

Where, n_i = moles of component i in the mixture and
c = number of components in the mixture

Note that the denominator is equal to the total number of moles of different substances present in the mixture. So the mole fraction of component i tells you what fraction of the total moles present in the mixture are the moles of this component i.

Example Problem 4-2

A mixture contains 25 kg of O_2. 30 kg of N_2 and 20 kg of NH_3. Find the mass fraction and mole fraction of each of the three components.

Solution

Mass fraction: The total mass, m = 25 + 30 + 20 = 75 kg The mass fractions, therefore, are

$$O_2, W_1 = \frac{25\, kg\, O_2}{75\ kg\ total} = 0.3333$$

$$N_2, W_2 = \frac{30\, kg\, N_2}{75\ kg\ total} = 0.4000$$

$$NH_3, W_3 = \frac{20\, kg\, NH_3}{75\ kg\ total} = 0.2667$$

For this three component system, w_3 may also be evaluated from:

$$w_3 = 1 - w_1 - w_2 = 0.2667.$$

Mole fraction: The molar masses are: O_2, M_1 = 32.00 kg/kmol; N_2, M_2 = 28.01 kg/kmol; NH_3, M_3 = 17.03 kg/kmol.
The numbers of moles are:

$$O_2, n_1 = \frac{25\ kg\ O_2}{32.0\ kg/kmol} = 0.7813\ kmol$$

$$N_2, n_2 = \frac{30\ kg\ N_2}{28.01\ kg/kmol} = 1.0710\ kmol$$

$$NH_3, n_3 = \frac{20\ kg\ NH_3}{17.03\ kg/kmol} = \frac{1.1744}{}\ .$$

Total 3.0267 kmol

Therefore,

$$x_1 = \frac{0.7813\ kmol\ O_2}{3.0267\ kmol\ total} = 0.2581$$

$$x_2 = \frac{1.0710\ kmol\ N_2}{3.0267\ kmol\ total} = 0.3539$$

$$x_3 = \frac{1.1744\ kmol\ NH_3}{3.0267\ kmol\ total} = 0.3880\ .$$

Again, as with mass fractions, x_3 may be determined from:

$$x_3 = 1 - x_1 - x_2 = 0.3880\ .$$

Volume-Fraction

Volume fraction of Component i in a Mixture containing c components is denoted by v_i and is defined as

$$v_i = \frac{V_i}{V_1 + V_2 + V_3 + - - - - + V_c}, \quad 1 \le i \le c$$

Where, V_i = volume of component i in the mixture and
c = number of components in the mixture

Note that the denominator is equal to the total volume of the mixture. So the volume fraction of component i tells you what fraction of the total volume of the mixture is composed of component i.

Useful observations on compositions

- Mass, mole or volume fractions define the composition of the mixture and are independent of the total size of the system.
- If you took a small portion out of a homogenous mixture, it will have the same composition, i.e. same mass fractions, same mole fractions and same volume fractions as existed in the original mixture.

If you take a small drop of beer from a keg, it has the same 5% alcohol by volume that the large keg had. Let us now consider an important question regarding compositions.

Can you specify mass-fractions of all c components in a mixture independently?

The answer is **NO**.

- You can specify mass-fractions of c-1 components, and that automatically fixes the mass fraction of the last component.
- The same can be said for the mole fractions and volume fractions also.

The volume fractions, mass fractions and mole fractions have to add to exact 1.0. Similarly, mass fractions and mole fractions have to add up to exact 1.0.

$$\sum_{i=1}^{c} W_i = W_1 + W_2 + W_3 + ----+ W_{c-1} + W_c$$

$$= \frac{m_1}{m_1 + ----+ m_c} + \frac{m_2}{m_1 + ----+ m_c} + \frac{m_3}{m_1 + ----+ m_c} + ----+ \frac{m_c}{m_1 + ----+ m_c}$$

$$= \frac{m_1 + m_2 + m_3 + ---+ m_c}{m_1 + m_2 + m_3 + ---+ m_c}$$

$$= 1.0$$

Or, $W_c = 1.0 - (W_1 + W_2 + W_3 + ----- + W_{c-1})$

Similarly, you can show that

$x_c = 1.0 - (x_1 + x_2 + x_3 + ----- + x_{c-1})$

and

$v_c = 1.0 - (v_1 + v_2 + v_3 + ----- + v_{c-1})$

Converting Mass Fractions to Mole Fractions

Often it becomes necessary to convert one type of compositions to another type. For example, you are given mass fractions but the equation that you want to use for something requires mole fractions. It is not that difficult to convert from one type to another if you remember the definitions of mass fraction and mole fraction and know how to convert mass of a substance to number of moles. The procedure for converting mass fractions to mole fractions can be outlined as:

1. Assume a convenient total mass, say 1 kg, of the mixture.
2. Calculate the mass of each component in the mixture by multiplying the total mass by the mass fraction.
3. Convert mass of each component to moles of that component by dividing by its molar mass.
4. Add all the moles to calculate total number of moles
5. Divide the number of moles of each component by the total number of moles to calculate the mole fractions.

Example Problem 4.3

A mixture contains 50% O2 and 50 % NH3.

(a) If the given composition is in mass percent, find the mole fractions.

(b) If the given composition is in mole percent, find the mass fractions.

Assume 1 kg of the mixture					
Component	Mass Fraction	Component Mass kg	Molar mass of the comp.	kmol of the component	Mole Fraction of the component
O_2	0.5	0.5	32	0.5/32 = 0.01563	0.01563/0.04499=0.3474
NH_3	0.5	0.5	17.03	0.5/17.03 = 0.02936	0.02936/0.04499=0.6526
Total	1.0	1		0.04499	1.0

Converting Mole fractions to Mass Fractions:

The procedure used is very similar. This time you start by assuming a total number of moles in the mixture and calculate the mass of each component for the assumed total moles. The procedure is

1. Assume a convenient total number of moles, say 1 kmol, of the mixture.
2. Calculate the moles of each component in the mixture by multiplying the total # of moles by the component mole fraction.
3. Convert number of moles of each component to mass of that component by multiplying by its molar mass.
4. Add all the mass values to calculate total mass of the mixture.
5. Divide the mass of each component by the total mass of the mixture to calculate the mass fractions.

Example Problem 4-3(b): Assume one kmol of the mixture					
Component	Mole Fraction	Component kmol	Molar mass of the comp.	Mass of the component	Mole Fraction of the component
O_2	0.5	0.5	32	0.5 x 32 = 16	16/24.52 = 0.653
NH_3	0.5	0.5	17.03	0.5 x 17.03 = 8.52	8.52/24.52 = 0.347
Total	1.0	1.0		24.52	1.0

Now that we have seen how it is done, we can write formal equations relating different types of compositions. For changing mass fractions to mole fractions:

$$x_j = \frac{W_j / M_j}{\sum_{i=1}^{c} W_i / M_i}$$

For changing mole fractions to mass fractions:

$$W_j = \frac{x_j \; M_j}{\sum_{i=1}^{c} x_i \, M_i}$$

For changing volume fractions to mass fractions, you need to convert volumes to mass. This is done by multiplying the volume of a component by its density. For converting volume fractions to mass fractions, the equation is

$$W_j = \frac{v_j \;\; \rho_j}{\sum_{i=1}^{c} v_i \;\; \rho_i}$$