Estimation of molecular weight knowing the mixture composition — and — Conversion of mole fraction to mass fraction and vice versa

1 Introduction

The article addresses two aspects pertaining to homogeneous gas phase systems composed of mixture of gases. The aspects addressed are;

1. Estimation of mixture molecular weight with the knowledge of
   - specie mole fraction in the mixture
   - specie mass fraction in the mixture
2. Estimation of
   - specie mass fraction knowing the mole fraction
   - specie mole fraction knowing the mass fraction

2 Nomenclature

n :	Number of gaseous species in the mixture
X_i :	Specie mole fraction
Y_i :	Specie mass fraction
MW_i :	Specie molecular weight
MW_{mix} :	Mixture molecular weight

3 Pre-requisite definitions:

$$\text{Molecular weight of a specie i} = MW_i = \frac{\text{Mass of specie i}}{\text{Moles of specie i}} \quad \left(\frac{kg}{kmole}\right)$$

$$\text{Molecular weight of mixture} = MW_{mix} = \frac{\text{Total mass of mixture}}{\text{Total moles of mixture}} \quad \left(\frac{kg}{kmole}\right)$$

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$$\text{Specie mole fraction in the mixture} = X_i = \frac{\text{Moles of specie 'i' in mixture}}{\text{Total moles of mixture}} \qquad \left(\frac{kmole}{kmole}\right)$$

$$\sum_{i=1}^{i=n} X_i = 1$$

$$\text{Specie mass fraction in the mixture} = Y_i = \frac{\text{Mass of specie 'i' in mixture}}{\text{Total mass of mixture}} \qquad \left(\frac{kg}{kg}\right)$$

$$\sum_{i=1}^{i=n} Y_i = 1$$

4 Estimation of mixture molecular weight $[MW_{mix}]$

4.1 Knowing the mole fraction $[X_i]$ of species

Consider a system containing a mixture with n gaseous species. The following discussion describes the estimation of mixture molecular weight if the mixture composition is known in terms of the specie mole fraction in the mixture.

Reviewing the definition of mixture molecular weight, the denominator requires the total moles of mixture. The total moles of mixture appears in the denominator of the specie mole fraction which is a known parameter. Taking the product of the specie mole fraction with specie molecular weight provides the ratio of mass of specie i to the total moles of mixture. Summing up the product for each specie for all the species in the mixture provides the mixture molecular weight. This is as presented below;

$$X_i * MW_i \longrightarrow \frac{\text{Moles of specie 'i' in mixture}}{\text{Total moles of mixture}} * \frac{\text{Mass of specie i}}{\text{Moles of specie i}}$$

$$X_i * MW_i \longrightarrow \frac{\cancel{\text{Moles of specie 'i' in mixture}}}{\text{Total moles of mixture}} * \frac{\text{Mass of specie i}}{\cancel{\text{Moles of specie i}}}$$

$$X_i * MW_i \longrightarrow \frac{\text{Mass of specie 'i' in mixture}}{\text{Total moles of mixture}}$$

$$\sum_{i=1}^{i=n} X_i * MW_i \longrightarrow \frac{\text{Mass of specie '1' in mixture}}{\text{Total moles of mixture}} + \frac{\text{Mass of specie '2' in mixture}}{\text{Total moles of mixture}} + ...$$

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$$\sum_{i=1}^{i=n} X_i * MW_i \longrightarrow \frac{\text{Total mass of mixture}}{\text{Total moles of mixture}}$$

Thus;

$$MW_{mix} = \sum_{i=1}^{i=n} X_i * MW_i$$

4.2 Knowing the mass fraction $[Y_i]$ of species

While the estimation of mixture molecular weight knowing the mole fraction was rather straight forward, estimation of the mixture molecular weight knowing the mass fraction has an additional step involved. This is described as below;

Reviewing the definition of specie mass fraction and specie molecular weight, mass fraction provides the total mass of mixture in the denominator. Taking the ratio of specie mass fraction to the specie molecular weight, we arrive at the ratio of moles of specie 'i' to the total mass of mixture. Summing over all the species provides the ratio of total moles of mixture to the total mass of mixture which basically the reciprocal of mixture molecular weight. This is presented as below;

$$\frac{Y_i}{MW_i} \longrightarrow \frac{\dfrac{\text{Mass of specie 'i' in mixture}}{\text{Total mass of mixture}}}{\dfrac{\text{Mass of specie i}}{\text{Moles of specie i}}}$$

$$\frac{Y_i}{MW_i} \longrightarrow \frac{\dfrac{\cancel{\text{Mass of specie 'i' in mixture}}}{\text{Total mass of mixture}}}{\dfrac{\cancel{\text{Mass of specie i}}}{\text{Moles of specie i}}}$$

$$\frac{Y_i}{MW_i} \longrightarrow \frac{\text{Moles of specie 'i' in mixture}}{\text{Total mass of mixture}}$$

$$\sum_{i=1}^{i=n} \frac{Y_i}{MW_i} \longrightarrow \frac{\text{Moles of specie 1 in mixture}}{\text{Total mass of mixture}} + \frac{\text{Moles of specie 2 in mixture}}{\text{Total mass of mixture}} + ...$$

$$\sum_{i=1}^{i=n} \frac{Y_i}{MW_i} \longrightarrow \frac{\text{Total moles of mixture}}{\text{Total mass of mixture}}$$

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$$\frac{1}{\sum_{i=1}^{i=n} \frac{Y_i}{MW_i}} \longrightarrow \frac{\text{Total mass of mixture}}{\text{Total moles of mixture}}$$

Thus;

$$MW_{mix} = \frac{1}{\sum_{i=1}^{i=n} \frac{Y_i}{MW_i}}$$

5 Conversion between mole fraction and mass fraction of species

5.1 Conversion from mole fraction to mass fraction

To arrive at

$$Y_i = \frac{\text{Mass of specie 'i' in mixture}}{\text{Total mass of mixture}}$$

knowing

$$X_i = \frac{\text{Moles of specie 'i' in mixture}}{\text{Total moles of mixture}}$$

First, divide the specie mole fraction X_i by the mixture molecular weight to ensure the desired denominator; the total mass of the mixture.

$$\frac{X_i}{MW_{mix}} \longrightarrow \frac{\frac{\text{Moles of specie 'i' in mixture}}{\cancel{\text{Total moles of mixture}}}}{\frac{\text{Total mass of mixture}}{\cancel{\text{Total moles of mixture}}}} \longrightarrow \frac{\text{Moles of specie 'i' in mixture}}{\text{Total mass of mixture}}$$

Multiplying the ratio of mole fraction and mixture molecular weight with specie molecular weight;

$$\frac{X_i}{MW_{mix}} * MW_i \longrightarrow \frac{\cancel{\text{Moles of specie 'i' in mixture}}}{\text{Total mass of mixture}} * \frac{\text{Mass of specie i}}{\cancel{\text{Moles of specie i}}} \longrightarrow Y_i$$

Thus;

$$Y_i = X_i * \frac{MW_i}{MW_{mix}}$$

5.2 Conversion from mass fraction to mole fraction

To arrive at

$$X_i = \frac{\text{Moles of specie 'i' in mixture}}{\text{Total moles of mixture}}$$

knowing

$$Y_i = \frac{\text{Mass of specie 'i' in mixture}}{\text{Total mass of mixture}}$$

First, multiple the specie mass fraction Y_i with the mixture molecular weight to ensure the desired denominator; the total moles of the mixture.

$$Y_i * MW_{mix} \longrightarrow \frac{\text{Mass of specie 'i' in mixture}}{\cancel{\text{Total mass of mixture}}} * \frac{\cancel{\text{Total mass of mixture}}}{\text{Total moles of mixture}}$$

$$Y_i * MW_{mix} \longrightarrow \frac{\text{Mass of specie 'i' in mixture}}{\text{Total moles of mixture}}$$

Dividing the mass fraction, mixture molecular weight product with the specie molecular weight, the specie mole fraction is obtained.

$$Y_i * \frac{MW_{mix}}{MW_i} \longrightarrow \frac{\cancel{\text{Mass of specie 'i' in mixture}}}{\text{Total moles of mixture}} \longrightarrow \frac{\text{Moles of specie 'i' in mixture}}{\text{Total moles of mixture}} \longrightarrow X_i$$

Thus;

$$X_i = Y_i * \frac{MW_{mix}}{MW_i}$$

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