Example Problem 1.1: Calculate the mass concentration of 2 gram moles of sulpher dioxide to be used to manufacture sulfuric acid in a 0.20 m3 of reactor.

Solution 1.1: 2 moles of sulpher dioxide is equal to $64 \times 2g = 128$ g

So mass concentration is $128\ g/0.20\ m^3 = 128 \times 0.001\ kg/0.20\ m^3 = 0.64\ kg/m^3$

Example Problem 1.2: A mixture of noble gases [helium, argon, krypton, and xenon] is at a total pressure of 100 kPa and a temperature of 200 K. If the mixture has equal kmole fractions of each of the gases, determine:

a) The composition of the mixture in terms of mass fractions.

b) Total molar concentration

c) The mass density.

Solution 1.2:

(a) Let 100 kmol of the mixture

Molecular weight of helium, argon, krypton (3), and xenon (4) are 4, 40, 83.8 and 131.3 kg/mol respectively.

Moles of each component of the mixture = 25 moles

So total mass of mixture = $25\times4+ 25\times40+25\times83.8+25\times131.3$ = 6477.5 kg

So mass fractions (component mass/ Total mass) are:

Helium = $25\times4/6477.5$ = 0.015,

Argon = $25\times40/6477.5$= 0.154,

Krypton = $25\times83.8/6477.5$ = 0.323 and

Xenon =$25\times131.3/6477.5$ = 0.507

The average molecular weight of the mixture = total mass/100 kmol = 6477.5 kg/100 kmol = 64.775 kg/kmol = 0.064775 kg/mol

(b) Temperature T = 200 K, Pressure P = 100 kPa, R = 8.314 kPa.m^3.kmol^{-1}.K^{-1}.
So Total molar concentration, C = P/RT = 60.14 mol/m^3.

(c) Mass density = Total molar concentration (C) $\times$ average molecular weight of the mixture = 60.14 mol/m^3$\times$0.064775 kg/mol = 3.896 kg/m^3.

1.2.2 Fluxes

The flux is defined as the rate of transport of species i per unit area in a direction normal to the transport. The flux is calculated with respect to a fixed reference frame. The molar flux of species i can be represented as

$$N_{i-mol} = C_i u_i \tag{1.10}$$

Here $N_{i\text{-}molar}$ is the molar flux of species i and u_i is the velocity of i with respect to a fixed reference frame. In the same fashion, a mass flux, $N_{i\text{-}mass}$ can be represented as

$$N_{i-mass} = \rho_i u_i \tag{1.11}$$

The units of the molar and mass fluxes are moles/m^2.s and mass/m^2.s. Sometimes it is convenient to interpret the total flux of species i with respect to an arbitrary reference frame rather than a fixed set of reference frame. The molar flux of species i based on arbitrary reference velocity u_0 is denoted by $J_{i\text{-}mol}$ which can be defined as

$$J_{i-mol} = C_i (u_i - u_0) \tag{1.12}$$

Similarly mass flux of species *i* based on arbitrary reference velocity u_0 is denoted by J_{i-mass} which can be expressed as

$$J_{i-mass} = \rho_i (u_i - u_0) \tag{1.13}$$

In a system, since several molecular species move with different average velocities, a frame of moving reference must be chosen. The important moving references are mass average, molar average and volume average velocities.

Mass-average velocity

The mass average velocity can be defined in terms of the mass concentration and the velocity of species *i* based on fixed axis. It is expressed as

$$U_{mass} = \frac{\sum_{i=1}^{n} \rho_i u_i}{\sum_{i=1}^{n} \rho_i} \qquad (1.14)$$

Molar average velocity

The molar average velocity can be expressed by the expression analogous to the mass average velocity. It can be represented by replacing mass concentration of species i, ρ_i with molar concentration of species *i*, C_i :

$$U_{mol} = \frac{\sum_{i=1}^{n} C_i u_i}{\sum_{i=1}^{n} C_i} \tag{1.15}$$

Volume average velocity

For experimental analysis the volume average velocity is important due to a fixed system of constant volume. The volume average velocity can be expressed by

$$U_{vol} = \sum_{i-1}^{n} \bar{v}_i C_i u_i \tag{1.16}$$

where $\bar{v}_i$ is the partial molar volume of species i.

Relation between fluxes

One can obtained the molar flux of i expressed in Equation (1.12) with respect to the molar average velocity as

$$J_{i-mol} = C_i\,(u_i - U_{mol}) \tag{1.17}$$

Substituting the Equation (1.10) into the Equation (1.17) and rearranging gibes

$$N_{i-mol} = J_{i-mol} + C_i U_{mol} \tag{1.18}$$

Again substituting the definition of molar average velocity defined in Equation (1.15) into the Equation (1.18) we get

$$N_{i-mol} = J_{i-mol} + C_i \frac{\sum_{i=1}^{n} C_i u_i}{\sum_{i=1}^{n} C_i} \tag{1.19}$$

Or

$$N_{i-mol} = J_{i-mol} + x_i \sum_{i=1}^{n} N_{i-mol} \tag{1.20}$$

For binary system of component A and B, $\sum_{i=1}^{n} N_{i-mol} = N_A + N_B = N$. Therefore the Equation (1.20) can be written for binary system as

$$N_{A-mol} = J_{A-mol} + x_A N \quad (1.21)$$

Example Problem 1.3: One kmole of gas mixture at a total pressure of 250 kPa and 303 K contains 10% CH_4, 30% C_2H_6, and 60% H_2 by volume. The absolute velocities of each species are -10 m/s, -5 m/s, and 15 m/s, respectively, all in the direction of the z-axis.

(a) Determine the molar average velocity, U_{mol} for the mixture.

(b) Evaluate the four fluxes: $J_{CH4-mol}$, $N_{CH4-mol}$.

Solution 1.3:

(a) $$U_{mol} = \frac{\sum_{i=1}^{n} C_i u_i}{\sum_{i=1}^{n} C_i} = \sum_{i=1}^{n} y_i u_i = (0.1)(-10) + (0.30)(-5) + (0.60)(15) = 6.5 \text{ m/s}$$

(b) C = P/RT = 250/(8.314*303) = 0.09924 kmol/m^3 = 99.24 mol/m^3

C_{CH4} = 0.10*99.24 mol/m^3 = 9.924 mol/m^3

$J_{CH4-mol} = C_{CH4}(u_{CH4} - U_{mol})$ = (9.924)*(-10-6.5) = -163.746 mol/m^{2}s

$N_{CH4-mol} = J_{CH4-mol} + C_{CH4} U_{mol}$ = -163.746 + 9.924*6.5 mol/m^{2}s = -99.24 mol/m^{2}s

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