Department of Chemical Engineering
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Course: Material and Energy Balances UCH301

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Mole fraction
Weight fraction
Stoichiometry and Chemical Equation

gram mole, pound mole, kmol

- While working on reacting systems or dealing with gaseous mixtures, molar units are commonly used.
- Many a times we need to convert mass units into moles units and vice-versa.
- gram mole (or moles) of a substance can be obtained by using the following relation:

  g-mole of a substance

  = mass in grams/molecular weight

  lb_m-moles of an elementary substance

  = mass in lb_m/molecular weight
- kmole of a substance

  = mass in kg/molecular weight

Mol fraction & Mass fraction

Mole fraction is the ratio of moles of a substance in a mixture (gas, liquid, solid) to the total moles of the mixture.

Mole fraction of A =   moles of A/(total moles)

Mass fraction is the ratio of mass of a substance in a mixture (gas, liquid, solid) to the total mass of the mixture.

Mass fraction of A =   mass of A/(total mass)

The sum of mol fractions/mass fractions of all components in a mixture is equal to 1.0

Excercise

- A gas stream contains 15 mol% water vapor, 15 mol% CO_2, 20 mol% CO, and 50 mol% N_2. Calculate composition on mass basis (calculate mass% composition).

Solution

Basis: 100 mole of gas mixture

For calculating the mass% of each, first calculate the mass of each component from the data of moles.

As we have chosen 100 mol as basis of our calculation, we get the moles of each component in feed as follows:

15 mol H_2O, 15 mol CO_2, 20 mol CO, 50 mol N_2

Mass of each component can be calculated as,

Mass of water vapor = 15*18 = 270 gm

Mass of CO_2 = 15*44 = 660 gm

Mass of CO = 20*28 = 560 gm

Mass of N_2 = 50*28 = 1400 gm

Total mass of the mixture = 270+660+560+1400 = 2890 gm

- ✔ wt% water vapor = (270/2890)*100 = 9.34
- ✔ wt% CO_2 = (660/2890)*100 = 22.84
- ✔ wt% CO = (560/2890)*100 = 19.38
- ✔ wt% N_2 = (1400/2890)*100 = 48.44

(Check: sum of wt % should be 100)

Specific gravity

- Specific gravity is the ratio of two densities,
  i.e., density of the substance to the density of a reference substance
  (Reference substance for liquids is water at 4^0C)

✔ **In some problem statements API gravity is given**

- American petroleum Institute (API) gravity is used in petroleum industry to magnify the scale (since there are several components in an oil fraction with very little difference in their densities).

- The formula to calculate API gravity from sp. Gravity (SG):

$$^{0}API = \frac{141.5}{sp\ gr} - 131.5$$

- Conversely, SG of petroleum liquids can be obtained from their API values:

$$SG\ at\ 60^{o}F = \frac{141.5}{API + 131.5}$$

Specific volume is the inverse of density.

Concentrations (amount of solute per specified amount of solvent or solution) may be expressed in mass/volume, moles/volume, ppm in a problem statement

Stoichiometry

Consider the following chemical equation:

$C_7H_{16} + 11O_2 \rightarrow 7CO_2 + 8H_2O$

- This equation tells us that, 1 mol of heptane is reacting with 11 moles of oxygen to give 7 moles of CO_2 and 8 moles of H_2O.
- 1 , 11, 7, and 8 are stoichiometric coefficients of $C_7H_{16,}$ $11O_{2,}$ $7CO_2$ respectively.
- From stoichiometric coefficients we can know the amount of one substance related to the other substance required/produced in a reaction.

Many a times in is required in process that one of the reactant is supplied in excess (due to design and operational limitations).

For the material balance calculations it is desired to know which reactant is in excess and how much is its excess than the requirement.

Excess Reactant: A reactant that is present in more quantity than required by the reaction stoichiometry. As its requirement depends on the quantity of other reactant(s).

Limiting Reactant:-A reactant that is present in smallest stoichiomeric proportion is limiting reactant.

Calculation of excess/limiting reactant

Excess of a reactant can be calculated as,

$$\%\text{Excess of reactant A} = \frac{moles\ of\ A\ in\ feed - moles\ of\ A\ required\ by\ stoichiometry}{moles\ of\ A\ required\ by\ stoichiometry} \times 100$$

Exercise

If 2 kg/s O_2 is used to burn the 1 kg/s C,

(i) Identify the excess and limiting reactants

(ii) Calculate % excess for the excess reactant

Solution

Reaction: $C + O_2 \rightarrow CO_2$

From the stoichiometry,

1 mole of C requires 1 mole of O_2

Moles of C present = 1/12 =0.0833

Moles of O_2 present = 2/32 =0.0625

0.0833 moles of C require 0.0833 moles of O_2

Thus, Excess reactant is C as it is more than required

Limiting reactant is O_2

- % excess of C = (0.0833-0.0625)/0.0625

  = 33.3

Degree of completion of a reaction

It is the percentage of the limiting reactant converted to other products.

Fractional conversion of A =

Moles of A reacted/ moles of A in feed

<u>Exercise</u>

The oxidation of ethylene to produce ethylene oxide is: $2C_2H_4 + O_2$ □ $2C_2H_4O$

A feed contains 100 kmol C_2H_4 and 100 kmol O_2. If the degree of completion is 50%, how much of each reactant and product is present at the end.

Solution

From the reaction stoichiometry:

2 mol of ethylene require 1 mol of oxygen

The quantities given in feed show that

Limiting reactant = C_2H_4, Excess = O_2

Now, 50 kmol of C_2H_4 are converted

Therefore, O_2 converted = 25 kmol

Moles of each component at the end are:

C_2H_4 = 100-50 = 50 kmol

O_2 = 100-25 = 75 kmol

C_2H_4O = 50 kmol