

**Department of Chemical Engineering  
Thapar Institute of 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<sub>m</sub>-moles of an elementary substance**  
= mass in lb<sub>m</sub>/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%  $\text{CO}_2$ , 20 mol% CO, and 50 mol%  $\text{N}_2$ . 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  $\text{H}_2\text{O}$ , 15 mol  $\text{CO}_2$ , 20 mol CO, 50 mol  $\text{N}_2$



Mass of each component can be calculated as,

$$\text{Mass of water vapor} = 15*18 = 270 \text{ gm}$$

$$\text{Mass of CO}_2 = 15*44 = 660 \text{ gm}$$

$$\text{Mass of CO} = 20*28 = 560 \text{ gm}$$

$$\text{Mass of N}_2 = 50*28 = 1400 \text{ gm}$$

$$\text{Total mass of the mixture} = 270+660+560+1400 = 2890 \text{ gm}$$

- ✓ wt% water vapor =  $(270/2890)*100 = 9.34$
- ✓ wt% CO<sub>2</sub> =  $(660/2890)*100 = 22.84$
- ✓ wt% CO =  $(560/2890)*100 = 19.38$
- ✓ wt% N<sub>2</sub> =  $(1400/2890)*100 = 48.44$

(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<sup>0</sup>C)

- ✓ 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):

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

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

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



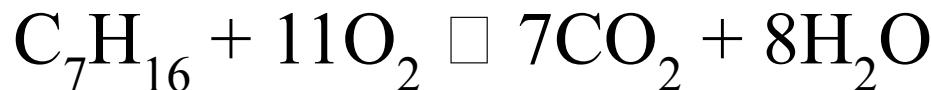
Specific volume is the inverse of density.

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:



- This equation tells us that, 1 mol of heptane is reacting with 11 moles of oxygen to give 7 moles of CO<sub>2</sub> and 8 moles of H<sub>2</sub>O.
- 1 , 11, 7, and 8 are stoichiometric coefficients of C<sub>7</sub>H<sub>16</sub>, 11O<sub>2</sub>, 7CO<sub>2</sub> 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 stoichiometric proportion is limiting reactant.



# Calculation of excess/limiting reactant

Excess of a reactant can be calculated as,

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

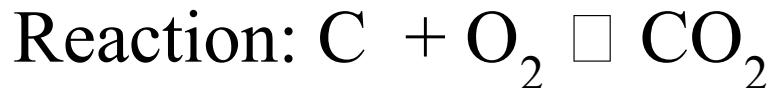
## Exercise

If 2 kg/s O<sub>2</sub> is used to burn the 1 kg/s C,

- (i) Identify the excess and limiting reactants
- (ii) Calculate % excess for the excess reactant



# Solution



From the stoichiometry,

1 mole of C requires 1 mole of O<sub>2</sub>

Moles of C present = 1/12 = 0.0833

Moles of O<sub>2</sub> present = 2/32 = 0.0625

0.0833 moles of C require 0.0833 moles of O<sub>2</sub>

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

**Limiting reactant is O<sub>2</sub>**

- % 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

## Exercise

The oxidation of ethylene to produce ethylene oxide is:  $2\text{C}_2\text{H}_4 + \text{O}_2 \rightarrow 2\text{C}_2\text{H}_4\text{O}$

A feed contains 100 kmol  $\text{C}_2\text{H}_4$  and 100 kmol  $\text{O}_2$ . 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 =  $\text{C}_2\text{H}_4$ , Excess =  $\text{O}_2$

Now, 50 kmol of  $\text{C}_2\text{H}_4$  are converted

Therefore,  $\text{O}_2$  converted = 25 kmol

Moles of each component at the end are:

$$\text{C}_2\text{H}_4 = 100 - 50 = 50 \text{ kmol}$$

$$\text{O}_2 = 100 - 25 = 75 \text{ kmol}$$

$$\text{C}_2\text{H}_4\text{O} = 50 \text{ kmol}$$

