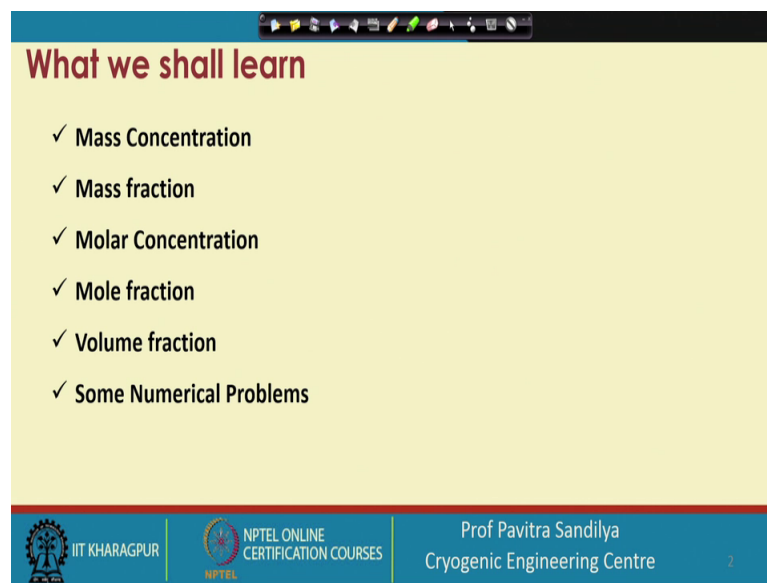


Upstream LNG Technology
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Lecture – 02
Concentration

Welcome back. Today we shall be looking into some fundamentals which are necessary for the analysis of the numerical problems, we shall be encountering later while we are learning about the various types of processes for the separation in the Upstream LNG Technology. So, today we shall be looking into the various ways of determining the concentration. Some of these concepts, you might have already learnt earlier we shall be just kind of recapitulating whatever you have learned.

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What we shall learn

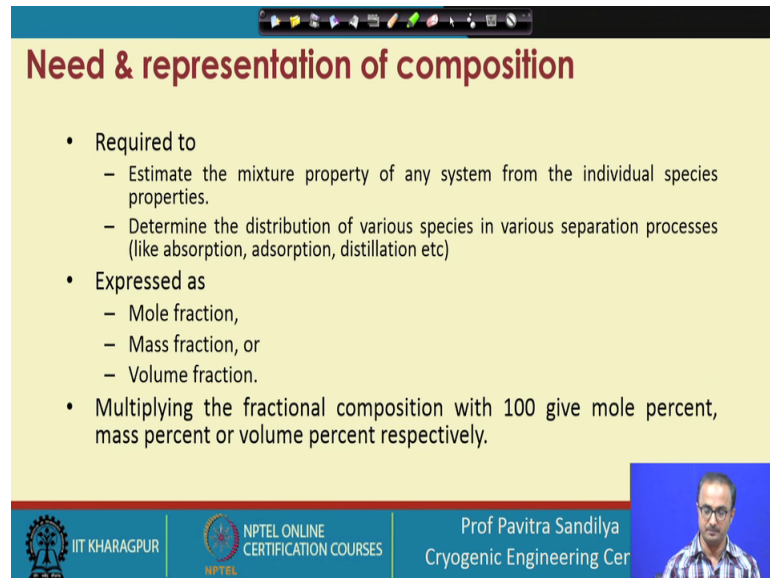
- ✓ Mass Concentration
- ✓ Mass fraction
- ✓ Molar Concentration
- ✓ Mole fraction
- ✓ Volume fraction
- ✓ Some Numerical Problems

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Today, first we shall see the various types of representation of the concentrations, these representations are not exhaustive there are many more representations, but we shall be looking into only those which we shall be using more often in the analysis. In this first comes the mass concentration, then comes the mass fraction molar concentration, mole fraction and volume fraction. After learning about these concentrations we shall be doing a few numerical problems to illustrate, how we shall be determining and converting these various types of concentrations. Let if you understood that even though this concentration may be in different types of units, different types of definitions, but it is

very much possible for us to convert one type of concentration to another type of concentration.

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Need & representation of composition

- Required to
 - Estimate the mixture property of any system from the individual species properties.
 - Determine the distribution of various species in various separation processes (like absorption, adsorption, distillation etc)
- Expressed as
 - Mole fraction,
 - Mass fraction, or
 - Volume fraction.
- Multiplying the fractional composition with 100 give mole percent, mass percent or volume percent respectively.

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Why do we need to give the concentrations? Now, then it is needed because we need to sometimes estimate the property of a mixture of any system, it may be gas, it liquid from the individual species properties. For example, we may be knowing the properties like thermal conductivity, density, viscosity, etcetera for individual species in a mixture, but when it comes to the determination of the properties of the mixture as a whole, then we would need the knowledge of the concentration of each of the species to determine the average property of the mixture under study.

And the second utility of concentration is that when we are learning and analyzing various types of processes, we need to know how each of the species is getting distributed in the system. Various species, they may be undergoing or may not be undergoing any kind of chemical reaction. And as per the process behavior, how the species are getting redistributed into the system. So, that from there, we can understand the performance and efficiency of a given system for all this, we need the knowledge of the composition which are given in terms of the concentration.

Now, the representations of the concentrations are there like mole fraction mass fractional volume fraction and when we are multiplying these fractions with 100, we get

the percentage; that means, if I multiply the mole fraction with 100, I get the mole percentage if I multiply mass fraction with hundred I get the mass percentage and so on.

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Mass Concentration

✓ Defined as the mass of a species per unit volume of a mixture

$$\omega_i \equiv \frac{m_i}{V}$$

Where ω_i is the mass concentration of species i ,
 m_i is the mass of species i and
 V is the volume of the mixture

✓ Dimension - ML^{-3}

SI unit: $\frac{Kg}{m^3}$, $\frac{g}{cm^3}$, $\frac{g}{l}$

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Now, first we come to the definition of mass concentration, the mass concentration is divide, they were defined as the mass of a species, but unit volume of a mixture and it is obtained by dividing the mass of a species which is given by m_i by the volume of the mixture that is given by V . And generally it is represented in terms of ω_i , but please note that you may find different types of representations of these various and definitions in different books or in different literature.

So, here I am using ω_i for mass concentration, next in line is the dimension the dimension means what kind of units we shall be having for and to represent these concentrations. Now for determine the units, we go back to our basic fundamental units like in case of concentration, it is coming in terms of the mass M and some length dimension that is given by L ; so, mass per length to the power 3. Now length to about three means it is volume. So, it is mass per unit volume.

So, in case of mass concentration if I represent in terms of the SI unit, it will be the SI unit will be kg per meter cube other than this, we may have other units to like we can have gram per centimeter cube or gram per liter. And depending on the unit system, we are using whether we are using SI system whether we are using mks system, whether we are using cgs system, we will be having different types of units for this concentration.

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Mass fraction

- ✓ Mass (or weight) fraction of species i ($\tilde{\omega}_i$) is defined as

$$\tilde{\omega}_i \equiv \frac{m_i}{\sum m_i}$$

- ✓ Dimensionless

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Next, we come to the definition of mass fraction. Now let us see, how we define the mass fraction. Mass fraction is defined like the mass of a given species that is m_i and the total mass in the system that is given by the sigma m_i that is we are simply adding the masses of all the species and it is given denoted by this omega i with a tilde. And because here it is a fraction and which is constituting of mass only in the numerator and denominator, it is dimensionless next in line is the molar concentration.

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Molar Concentration

- ✓ Defined as the number of moles of a species per unit volume of a mixture

$$c_i \equiv \frac{n_i}{V}$$

- ✓ Dimension - ML^{-3}

$\frac{mol}{m^3}$ $\frac{mol}{l}$

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The molar concentration is given by c_i where it is defined as the number of moles of a species i divided by the volume of the mixture and when it comes to its dimension, the dimension is again m per l cube; that means, it is again this m; m here stands for the amount of the particular species the amount may be given in terms of mass like kg, gram, etcetera or it may also be given in terms of the number of moles. So, in case of molar concentration, the unit may be mol per meter cube or moles per liter and so on and so forth. So, we shall be using this kind of units for molar concentration.

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Mole fraction & Volume fraction

- ✓ Mole fraction (y_i) of a species i in a mixture is defined as

$$y_i \equiv \frac{n_i}{\sum n_j}$$
 where n_i is the number of moles of species i in the mixture
- ✓ Volume fraction of a species i in a mixture is defined as

$$(\text{volume fraction})_i \equiv \frac{v_i}{V}$$

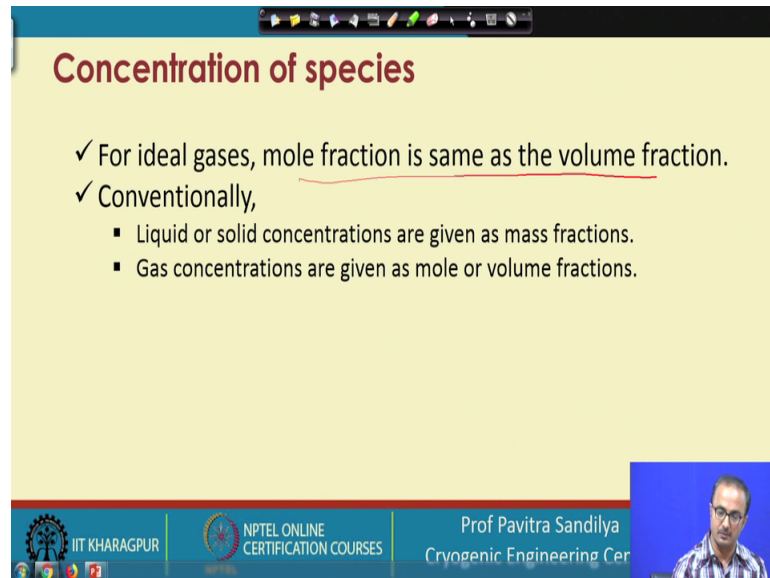
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Next is line is mole fraction and volume fraction. Now, first let us see, what is mole fraction mole fraction analogous to mass fraction is defined as the number of moles of a species i divided by the total number of moles present in the mixture. And this is denoted by a notation say y_i in general this y_i represents the molar fraction of a species in vapor state and for a liquid state we generally use x_i , but here we are just sticking to y_i for definition of the mole fraction.

Now, volume fraction is defined as the volume occupied by a given species i divided by the total volume of the mixture. Now in this case, please note I have not put the total volume in terms of summation of the individual volumes because of the fact that volume is not in general conserved unlike mass, we have different types of system ideal system non ideal system about which we shall be learning later which may or may not give the total volume from the addition of the individual volumes the addition of individual

volumes leads to total volume only in case of ideal system or ideal liquids, but not in case of non ideal systems. So, that is why, I have not put the total volume as the summation of the species volumes.

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Concentration of species

- ✓ For ideal gases, mole fraction is same as the volume fraction.
- ✓ Conventionally,
 - Liquid or solid concentrations are given as mass fractions.
 - Gas concentrations are given as mole or volume fractions.

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The two points that when we talk of ideal gases we have the mole fraction is same as the volume fraction and this can be easily proved considering the ideal gas equation of state and conventionally the liquid or the solid concentrations are given in terms of the mass fractions while the gas concentrations are given in terms of the mole or volume fractions. So, if nothing is mentioned in a given problem we shall be go by the convention.

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Average or Apparent Molecular weight

- Used for mixtures like liquid solutions, natural gas, air etc.
- Determined as mole fraction average of the molecular weights of all components in the mixture.

$$M_a = \sum_{i=1}^{n_c} y_i M_i$$

Where M_a is the average molecular weight, n_c is the total number of components, y_i is the mole fraction of species i , and M_i is the molecular weight of species i .

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After knowing these concentration units, let us go to the calculation of the average or apparent molecular weight. Now why do we need it because we need it for knowing the concentrations of the mixture like liquid solutions and gases and in natural gas especially we have so many types of components depending on the types of components?

We will be having different molecular weight or apparent molecular weight of natural gas and this thing is determined by the following definition that the average molecular weight which is given by M_a is taken as some average that is the we call it the mole fraction weighted average of the individual molecular masses. In this case, you can see that y_i is the mole fraction of the species i whereas, M_i is the molecular mass of species i and this is being summed up for species 1 2 n_c where n_c represents the total number of species present in the particular system.

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• Other representations of concentration

- Molarity
- Molality
- Normality etc.

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There may be other representations of concentration like molarity, molality, normality, etcetera which I shall not be mentioning in this, but as then when the cases come up, we shall be talking about these types of units.

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Conversion of mole fraction to mass fraction

y_i = mole fraction of species i
 $\tilde{\omega}_i$ = mass fraction of species i
 n_i = number of moles of species i
 m_i = mass of species i
 M_i = molecular mass of species i
 M_a = average molecular mass of the mixture

$$y_i = \frac{n_i}{\sum_i n_i} = \frac{\frac{m_i}{M_i}}{\frac{\sum m_i}{M_a}}$$
$$\frac{m_i}{M_i} = y_i \frac{\sum m_i}{M_a}$$
$$\Rightarrow \frac{m_i}{\sum m_i} = y_i \frac{M_i}{M_a}$$
$$\frac{m_i}{\sum m_i} = \tilde{\omega}_i$$
$$\Rightarrow \tilde{\omega}_i = y_i \frac{M_i}{M_a}$$

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Now, let us see that how do we convert mole fraction to mass fraction first again we capitulate that whatever we have seen so far the notations that y_i stands for the mole fraction of species i , the $\tilde{\omega}_i$ is for the mass fraction of species i ; n_i is the number of moles of species i ; m_i is thus mass of species i capital M_i is the molecular

mass of species i and capital M with a subscript a is the average molecular mass of the mixture.

Now let us go with the basic definition of the mole fraction y_i here, we are writing the basic definition that is n_i divided by the total number of moles. Now, this n_i is now being put in terms of the ratio of the mass of the species i divided by its molecular weight that is capital M_i and we are representing the total number of moles in the system as the total mass in the system divided by the average molecular mass in the system.

Now, we will do some mathematical manipulation in this to see that we are writing this n_i by m_i is equal to y_i into summation of m_i divided by capital M_a and now, we shall see that with this mathematical manipulation, we have done and again we will see that that we have this definition of the mass fraction with this definition, we put it back into this equation and we get this particular equation. So, this equation gives us the relationship between the mass fraction and the mole fraction and we shall be needing this kind of conversion unit conversions many a times in our future analysis ok.

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1. Estimate the number of moles of methane in 1 kg of the gas.

Given: Mass of methane (CH_4) = 1 kg
Molecular mass of CH_4 = 16 kg/kmol

$$n_{\text{CH}_4} = \frac{1 \text{ kg}}{16 \text{ kg/kmol}} = 0.0625 \text{ kmol}$$

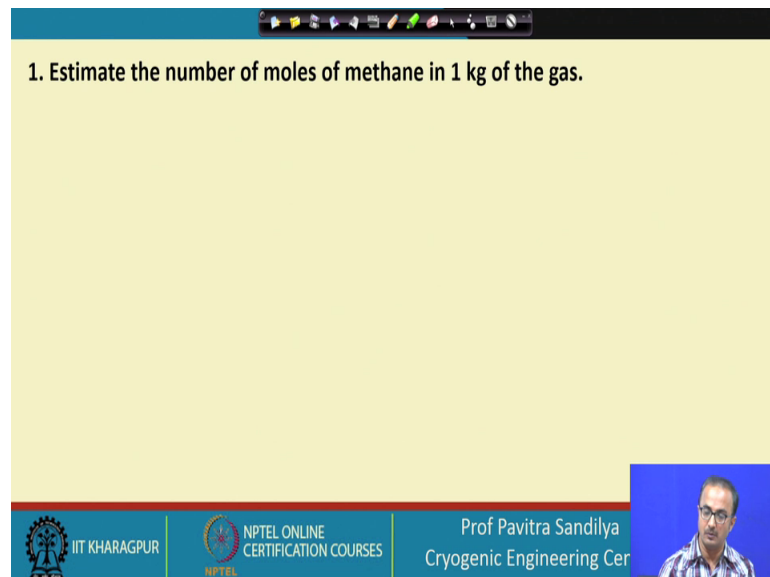
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Now, let us take up a problem to demonstrate the fundamentals we have learned so far; the first problem is like to estimate the number of moles of methane in 1 kg of the gas to solve this problem. Let us do let us see; how we do it first let us see; what is given to us given is mass of methane that is CH_4 is equal to 1 kg to convert it to the number of

moles, we need the molecular mass of methane and that is equal to 16 and its unit will be say kg per kilo mole, it may also be given in terms of gram per mole.

Now, because we are using the mass of methane in terms of kg; so, we are using the molecular mass also in terms of kg per kilo mole. Now from this the number of moles of methane is equal to the mass of methane divided by the molecular mass and this will give something with kilo mole. So, this value will be the kilo mole of methane in the particular mixture. So, this is how we calculate the number of moles of a species in a pure component.

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1. Estimate the number of moles of methane in 1 kg of the gas.

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2. Natural gas contains methane, ethane and propane in the mole percentages of 70, 20 and 10 respectively. Find

a. The average molecular weight of this natural gas.

b. The mass of each of the species in 1 kg of natural gas.

$$M_a = \sum y_i M_i$$
$$M_a = 0.7 \times 16 + 0.2 \times 30 + 0.1 \times 44 = \text{○} \text{ kg/kmol or g/mol}$$
$$M_{\text{CH}_4} = 16 \text{ kg/kmol}$$
$$M_{\text{C}_2\text{H}_6} = 12 \times 2 + 6 = 30 \text{ kg/kmol}$$
$$M_{\text{C}_3\text{H}_8} = 12 \times 3 + 8 = 44 \text{ kg/kmol}$$

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Next we go to another problem, now in this problem, we have been given the typical composition of natural gas consisting of methane ethane and propane and the composition have been given in terms of mole percentage that is 70 percent of methane, 20 percent of ethane and 10 percent of propane. Now please mind it that the summation of these mole percentage must always be adding up to hundred and the summation of the mole fractions or mass fractions must always be adding up to unity that is one.

Now, with this given information we have been asked to determine the average molecular weight of the natural gas and the mass of each species in 1 kg of natural gas. First let us go to the first problem average molecular weight of the natural gas, let us see, how to do it. The definition of the average molecular weight M_a was given as the summation of y_i into the capital M_i . Now in this case, the M_{CH_4} is 16 say kg per kilo mole, then $M_{\text{C}_2\text{H}_6}$ that is the ethane. Ethane is 12 into 2 plus 6; that is 24 plus 6 is 30 kg per kilo mole and propane is C_3H_8 that is 12 into 3 plus 8; that is 44 kg per kilo mole, I am sorry, there is a mistake here that ethane is C_2H_6 not H_4 ; that is 6 and this will be 6 here. So, it will be 30. So, be careful about writing these values.

Now, once we know the values; what we shall do to we shall find the average molecular weight as M_a is equal to 0.7 ; that is 70 by 100 . 0.7 into 16 plus 0.2 into 30 plus 0.1 into 44 . So, that is how we find the average molecular weight and again, it will be given with some

value in kg per kilo mole or it is same as gram per mole same. So, that is how we have solved the first part.

Now, let us go to the second part, in the second part, we have been asked to find the mass of each of the species in 1 kg of natural gas now because we have been given the 1 kg of natural gas, we have to find the how much is equivalent mass fraction of each of the species because the mass of each species is equal to mass fraction of the species into its molecular mass. So, we first need to convert the mole fractions into mass fractions and for that you can go back to the earlier definition of the inter conversion of mass and mole fraction and what you find that we have $\omega_i = y_i M_i / M_a$.

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2. Natural gas contains methane, ethane and propane in the mole percentages of 70, 20 and 10 respectively. Find

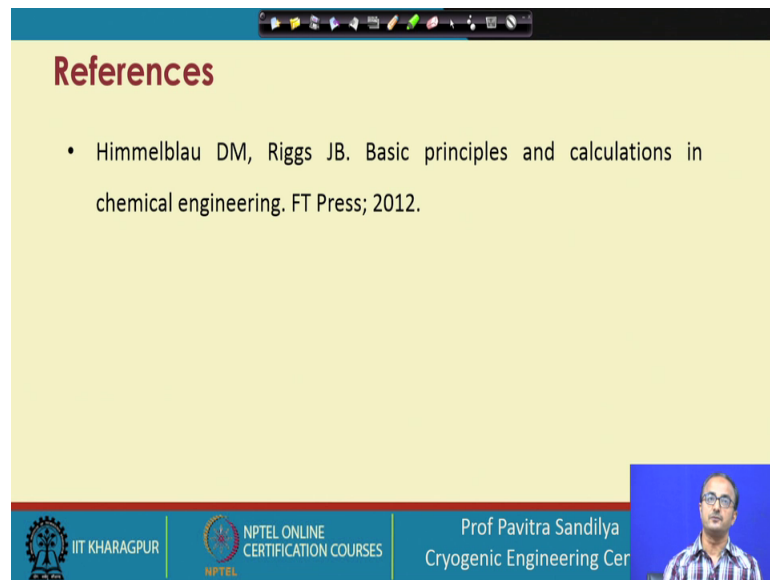
- The average molecular weight of this natural gas.
- The mass of each of the species in 1 kg of natural gas.

$$\omega_i = y_i \frac{M_i}{M_a}$$
$$m_i = \omega_i \times M_a$$

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Now, you see; in this case, everything is known to you know y_i you know M_i and you have determined M_a , earlier, you plug in the values you get the value of the ω_i and the mass of each species will be equal to now ω_i into the molecular mass and this will give you the mass of each species in one kg of the natural gas mixture. So, I hope that now if we proceed to other problems.

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References

- Himmelblau DM, Riggs JB. Basic principles and calculations in chemical engineering. FT Press; 2012.

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We can do it and for this you can refer to this book Himmelblau and Riggs basic principles and calculations in chemical engineering is a very wonderful book and you can learn all these fundamentals from this book.

Thank you.