

Material and Energy Balance Computations
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Lecture –05
Introduction to Processes and Process Variables (Contd.,)

Hello everyone, and welcome back once again in the final lecture of module 1 on Material and Energy Balance Computations where we were discussing the process variables.

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The slide is titled "Chemical Composition" and contains the following content:

- Mass fraction (x)
 - mass of a species / total mass of mixture
- Mole fraction (y)
 - moles of a species / total moles of mixture

Handwritten notes in red and blue ink include:

- A box containing: $x_A = 0.15$ and $y_B = 0.20$
- Text: "for 175 kg solution", "mass of A = 175 x 0.15 kg = 26 kg A"
- Text: "for the solution flow rate of 1000 ml/min", "molar flow rate of B = 200 ml B/min"
- A diagram showing a box with 'A' and 'B' inside, and a circle with 'y_i' above it.
- A small video inset of the professor in the bottom right corner.
- Logos of IIT Kharagpur and the Department of Chemical Engineering at the bottom.

So here we stopped at this point with the concept of mass and mole fraction. Now the mass fraction as I mentioned earlier is the mass of a species per total mass of the mixture. And the mole fraction is the moles of an individual species with respect to the total number of moles that is there in the mixture. The reason here it is mentioned x and this is y is because this is a typical convention that we express the mass fraction by x , say for example if there the component is the i^{th} component and its mass fraction is known we typically write that as x_i .

And the mole fraction we typically write for the i^{th} component is the y_i . This is a convention that we follow in this set of lecture. So the point is that these concepts or this understanding of the change of the conversion between the mass fraction and mole fraction is useful when we have the mixture and that is frequent in our future classes. So for example the information is given in such a way that we have the mass fraction of component A.

Say we have a mixture where component A and component B are there. The information given is that the mass fraction of A, which is x_A is 0.15 and mole fraction of B is 0.2 or in other words, you may find this problem statement like this that A is present 15% by mass and B is present as 20% by mole, which we can write in this way that x_A is 0.15 and y_B is 0.2. So, now so the total mass of the solution or the mixture is given, then we can easily find what is the mass of the A because we know its mass fraction multiplied by the total mass is the amount of A, which means the rest is component B by mass.


And say it is further mentioned that this solution is flowing at the rate of 1000 mol/min. So what is the flow rate of B or the molar flow rate of component B? That becomes 1000×0.2 which is 200 mol/min. Now such quick conversions or understanding of this information are necessary while computing our material and energy balance.

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Mass & Molar Composition 100g air

Component <i>i</i>	Mass Fraction $x_i = \frac{m_i}{m_{total}}$	Mass (g) $m_i = x_i m_{total}$	Molecular Weight M_i (g/mol)	Moles $n_i = \frac{m_i}{M_i}$	Mole Fraction $y_i = \frac{n_i}{n_{total}}$
O ₂	0.16	16	32	0.50	0.15
CO	0.04	4	28	0.14	0.04
CO ₂	0.17	17	44	0.39	0.12
N ₂	0.63	63	28	2.25	0.69
Total	1.00	100		3.28	1.00

Handwritten notes:
 Basis of Calculation
 100g air
 O₂ - 16%
 CO - 4%
 CO₂ - 17%
 N₂ - 63%
 Total Moles = 3.28



Now say it is mentioned the air the usual composition or the typical composition of air by mass, it is given like this that we have O₂ as 16% by mass so all these compositions are mentioned by mass. So CO carbon monoxide in air is around 4%, carbon dioxide is 17%, and nitrogen is 63% which is the major component of air by mass. So our task is to convert this information into the mole fraction. So there is a typical example that you can follow while converting this and how do you do that?

So we say for simplicity we form a table, where we write the components that are there. We write their mass fraction because this is given in percentage. So, the mass fraction for O₂, carbon monoxide, CO₂, nitrogen everything is taken from this information and we cross-check that indeed the total mass fraction should be 1. This is the cross-check you should do after or before the conversions for both mass and mole fractions.

Because it is a fraction, so the summation of all the fractions should be 1, which has to conserve. So that means now what is the mass of those species and individual species in the mixture, but here it is not mentioned how much or what is the amount of air that is given? In such cases and we will see that such cases are also very frequent. In those cases, we introduce the term called the basis of calculation. Based on some assumed value, say the amount of air we need to convert this information to the mole fraction and the result will be independent of this basis of calculation.

So it is the basis of calculation and that is assumed in order to simplify the calculation whichever is convenient. And here the convenience is that it is the mass fraction mentioned. So the logical assumption can be or it should be that we have either 100 g or 100 kg of air, and since here we are mentioning it in terms of g/mol. Let us assume we have 100 g of air. So, which means mass fraction multiplied by this total mass is the individual mass of the species? Again we can cross-check after converting that the total mass is indeed 100 grams?

We know the molecular weight of those individual species. Now, these things you have to remember because these are the fundamental things and you are aware of these things since + 2 level. So here we have 32 for oxygen, 28 for carbon monoxide, 44 for Carbon dioxide and 28 for nitrogen, these are the molecular weight that means the number of moles would be our mass divided by the molecular weight which is small m we have designated for mass, capital M for the molecular weight.

So, the number of mole is small m by capital M , we do it for respective cells and we get this value. Now, Remember our task is to convert the mass fraction to the mole fraction. So the mole

fraction is basically the ratio or the amount or the number of moles of the individual species with respect to the total number of moles of the mixture. So that means we need to calculate what is the total number of moles that is the summation of all 4 species, the number of moles.

And then we divide this individual species the n_i by the total mole. So it is n_i divided by the n_{total} , so that means $0.50/3.28$, the result is 0.15 . Here again, the essence of significant figures is preserved. So we do it for each and every species, and then if you remember in one of the lectures, I mentioned how do you realise or how do you understand that your calculations are correct?

Now here the logical state is that now I add all the 4 mole fractions and check whether it is indeed 1 or not because that has to be, and in this case, it is indeed the case. So from the mass fraction, we have converted to the mole fraction. So for any mixture, I hope you would be able to convert such information from either from mole fraction to mass fraction or mass fraction to mole fraction with the help of this information or this information.

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Average Molecular Weight

- Ratio of mixture mass and number of moles of all species

$$\bar{M} = y_1 M_1 + y_2 M_2 + \dots = \sum y_i M_i$$

$$\frac{1}{\bar{M}} = \frac{x_1}{M_1} + \frac{x_2}{M_2} + \dots = \sum \frac{x_i}{M_i}$$

Molar composition: 79% N_2 & 21% O_2
 Mass composition: 76.7% N_2 & 23.3% O_2

$$\begin{aligned} \bar{M} &= y_{N_2} M_{N_2} + y_{O_2} M_{O_2} \\ &= 0.79 \times 28 + 0.21 \times 32 \\ &= 29 \frac{\text{kg}}{\text{kmol}} \end{aligned}$$

So, the average molecular weight and it is essential for defining a mixture is the ratio of mixture mass and the number of moles of all species. So, for example, say we have components 1, 2, 3 these are the number of species we have. So if we have the information either based on their mass fraction or mole fraction, we should be able to calculate the mixtures mean or the average

molecular weight by such expression that this deals with the information on mole fraction it is y .

Now, from now on what we remember is that y means the mole fraction x means the mass fraction. So the bar represents the average value. So it is the summation of individual mole fraction multiplied by their respective molecular weight and the summation of all the species that would give me the value of the average molecular weight of a mixture. If the information is known based on the mass fraction, this is the expression we can use to calculate the value of the average molecular weight of that whole mixture.

So let's take an example say air again it mostly consists of Nitrogen and oxygen. So when it is typically not mentioned like in the previous example we have seen the carbon dioxide, carbon monoxide all these information's were given. If those are not mentioned, typical air composition we consider as 79% nitrogen and 21% oxygen by moles and in mass composition the same information can be used which is given here that is 76.7% nitrogen and 23.3% oxygen.

And let me tell you here itself that in several problems later when will solve it this molar composition of air would typically not be given because it is imperative that when such compositions are explicitly not mentioned you should assume that year consists of Nitrogen and oxygen by 79% and 21% mole fraction of Nitrogen and oxygen respectively. So now say we have this information and we have to find out what is the average molecular weight of air.

So quite logically if we apply the first equation, because here we have both the information so will cross-check our calculation or will see whether it leads to the same result or not. So in the first expression now, the Average molecular weight of air = (the mole fraction of Nitrogen \times molecular weight of Nitrogen) + (the mole fraction of oxygen \times the molecular weight of oxygen).

Which means from this is information that is given here; we write this expression and find out what is the average molecular weight.

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Average Molecular Weight

- Ratio of mixture mass and number of moles of all species

$$\bar{M} = y_1 M_1 + y_2 M_2 + \dots = \sum y_i M_i$$

$$\frac{1}{\bar{M}} = \frac{x_1}{M_1} + \frac{x_2}{M_2} + \dots = \sum \frac{x_i}{M_i}$$

Molar composition: 79% N₂ & 21% O₂
Mass Composition: 76.7% N₂ & 23.3% O₂

$$\frac{1}{\bar{M}} = \left(\frac{0.767}{28} + \frac{0.233}{32} \right) \frac{\text{mol}}{\text{g}}$$

$$= 0.035 \frac{\text{mol}}{\text{g}}$$

$$\Rightarrow \bar{M} = 29 \frac{\text{g}}{\text{mol}}$$

Now if we try to use the second expression because the mass composition is mentioned. So, any one of these would be given to you, and you have to calculate so the average molecular weight of that mixture. If you use the second expression here now, we see the similar result would be achieved. So here the average molecular weight of air based on the assumption as I mentioned if it is not mentioned explicitly such kind of composition.

It is 79% nitrogen and 21% oxygen that gives me the average molecular weight of air is 29 g/mol.

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Concentration

- Mass and Molar concentration

- mass and number of moles per unit volume of the mixture
- **molarity** - molar concentration of the solute in gram-moles solute/liter solution
- parts per million (ppm) and parts per billion (ppb)
 - parts (grams, moles) of the species per million or billion parts
 - used for trace species
 - $\text{ppm} = y \times 10^6$
 - $\text{ppb} = y \times 10^9$

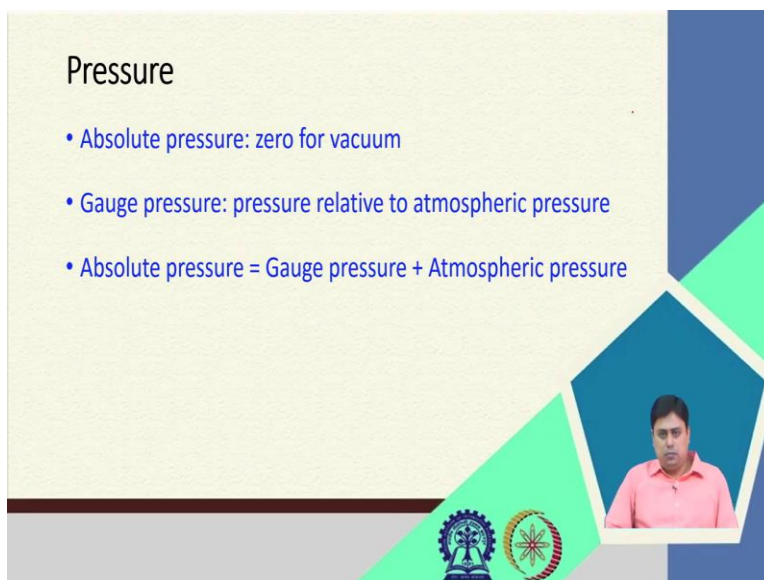
The other important concept that we should remember is the mass and molar concentration.

Those are the mass and the number of moles per unit volume of the mixture, respectively. That is the mass per unit volume is the mass concentration. The number of moles per unit volume is the molar concentration. We often hear the unit molarity in several places the molarity is the molar concentration of the solute in gram moles of solute per litre of the solution.

And now the term that I introduced earlier was the PPM and PPB which is the parts per million and parts per billion. These are the information given when there are trace species or trace amounts of species is present that are defined like this that it is the parts, parts means either gram, moles or whatever the consistent unit that you use in order to find the concentration is that the amount of that species per million or billion parts of those that mixture of the solution. If it is a million, then we say it is PPM. If it is per billion it is we say the PPB.

So, PPM is basically the mole fraction $\times 10^6$ and PPB is the mole fraction $\times 10^9$. So that means if I say that 15 PPM of sulphur dioxide is present in the air, that means we have 15 parts of SO_2 in a million parts of air. Now parts if you replace that with grams, that means 15 grams of SO_2 in 1 million grams of air and that is why you can now understand if you try to write that g/g of air, in scientific notation how many zeros are there in 10^{-6} , this kind of amount of zero will be involved. And when it is PPB, it is basically 10^9 is per billion of that air.

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Pressure

- Absolute pressure: zero for vacuum
- Gauge pressure: pressure relative to atmospheric pressure
- Absolute pressure = Gauge pressure + Atmospheric pressure

The other concept that we should refresh our memory is the understanding of the relation

between these 3 pressure terms is the absolute pressure, gauge pressure and atmospheric pressure. Absolute pressure comes with the reference that in a perfect vacuum the pressure is zero. That is the absolute pressure for that vacuum, this is the reference. Now, the gauge pressure because when we try to measure the pressure by a different devices pressure gauge.

So there the pressure is relative to the atmospheric pressure, which means if the gauge pressure is mentioned in a problem statement, we should be able to convert that to absolute pressure by adding gauge pressure with the atmospheric pressure, which means $\text{Absolute pressure} = \text{Gauge pressure} + \text{Atmospheric pressure}$. So sometimes in the problem statement, the absolute pressure is mentioned, we can find out easily what would be the gauge pressure.

So which means what we have done in these last couple of 4 and including this fifth lecture is that we understood several concepts, the very basic concepts, the purpose is to refresh your memory on several aspects. In addition to this pressure, concentration, mass density, specific gravity, say specific volume. There are other things that I have not mentioned assuming that those are pretty much you are familiar with those terms.

For example, say the force, the conversion of force in different units, those knowledge are necessary and would be utilized in the other lectures. There is say the temperature. Now it is pretty obvious that you should be aware of converting centigrade, Fahrenheit and say the Kelvin. So, if the information is given in centigrade or Fahrenheit, you should be able to convert that to Kelvin or vice versa.

So today what we have understood is the different process variables that encompass from the mass composition, molar composition their conversion in between those 2 types of composition. The pressure, the concentration and dimension there would be force, temperature. These actually are the components of different process variables. Now during our calculation these process variables we have to clearly identify.

We have to see their changes and if those are in, different or inconsistent units. We have to make it consistent. And remember that in this module, the take-home message is that any valid

equation should be dimensionally homogeneous. So while you write that expression check its dimensional homogeneity. During calculation see for unit consistency and use the conversion factors properly.

So with this, we conclude this module 1, and we will see in module 2 the Fundamentals of Material Balance, till then, thank you for your attention.