Material and Energy Balance Computations
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Lecture –04
Introduction to Processes and Process Variables

Hello everyone. Welcome back once again in the fourth lecture of Material and Energy Balance Computations. We are in the module that is an introduction to engineering calculations process and process variables. So in the last three lectures, we have covered the basics of units, dimensions, and the necessity of dimensional homogeneity. Today we will see what are actually processes and the utility of process variables.

Because for any calculation, any process calculation, first of all, we need to understand, what is the process? What are the parameters that are involved in the calculations and their conversion?

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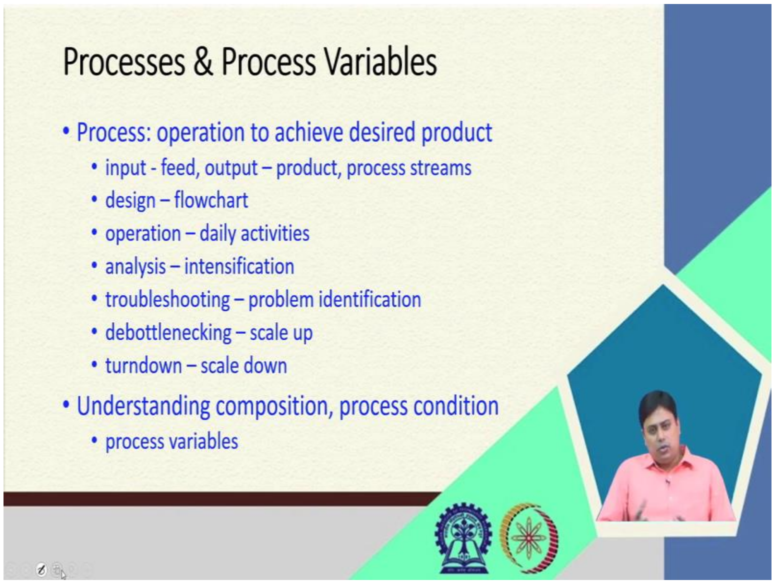

Processes & Process Variables

- Process: operation to achieve desired product
  - input - feed, output – product, process streams
  - design – flowchart
  - operation – daily activities
  - analysis – intensification
  - troubleshooting – problem identification
  - debottlenecking – scale up
  - turndown – scale down
- Understanding composition, process condition
  - process variables

So a process if we try to define, simply we can say it is an operation or stages of operation. Where we try to achieve some desired product that means it would have an input and an output, and technically these are called feed and the product, respectively. So input, we do not say typically input in the process calculation we say the feed that comes in when we try to convert that feed to some output and here the output is the product.

This flow of this inlet and outlet or say the feed and the product these are called the process streams. Now, as a process engineer, there would be some jargons, you will hear a couple of terms that we must be aware of. So, for example, that some people would be involved in designing a process that includes the formation of the layout. That will tell us that which operations need to be done after a certain operations or which one would precede in a certain stage of operation.

The sequence or the flow chart or the flow diagram is actually included in this design part. There are some engineers who are dealing with the process operations. So this process operation is nothing but its day to day activities so that the plant operates smoothly. So, this day to day activity, its maintenance and everything is included in the process operation. In addition to these two, say the design and operation we also have analysis.

Sometimes you have to do process analysis, or you have to analyse a process in order to intensify the operation; intensify means to enhance the rate of production. In order to do so, you have to add first understand and analyse the process, and then you may suggest some recommendations or recommended stages of operations, which can be included in the final stage. So while doing this analysis, there are certain stages as well or in fact during the operations.

Now, these are basically coupled, it is something that it is not you can single out. Why implementing a certain design idea you have to understand its operations and the operational difficulties. Now say there is a problem in a running plant that in several stages of operations where we are having some feed converted to the output, there are now certain problems when we try to identify or single out the problem that strategy of that process of the pathway we call the troubleshooting the problem.

These are the technical jargons, you should be aware of. So troubleshooting is the problem identification that means where the changes need to be done in order to get back to whatever we are having in a normal operation. Now say during the time of high demand of that certain product which we are producing in certain operations or stages of operations, we have to ramp up our production.

So, for example, in this kind of pandemic scenario that we are having since 2019-2021, in this period, there are certain industries, for example, medical pharmaceutical industries they need to ramp up their certain products production. Now when we try to do that, that is the stages that we need to scale up our production and that for that whatever we need to do. We need to understand we need to intensify a certain operation is called the debottlenecking operation, or the debottlenecking.

And when the demand is lower, the plant should still operate normally, but then that much amount of the production rate may not be necessary, so we need to scale down our production rate or reduce the production rate, that is called the turndown. So that means we have a process where there are several stages of operation happening in a typical commercial process, there is no such as commercial process where only single-stage operation is sufficient.

But for the sake of understanding a process, we can consider that even if a single operation is happening. That is a process that converts the feed to the product. Now the point is that, if we try to do any of the above things, that is the operation analysis, troubleshooting, debottlenecking, turndown whatever these, in fact, the design. So we need to understand what is the composition of the feed the product that we are looking for and the process condition in which the production can be optimised, the desired product we have to achieve.

So while producing a product, there can be several by-products as well which are not necessary, but you cannot avoid those. So our aim would be to reduce those by-products and increase or optimise the production of the desired products. For that, we need to understand the composition of the feed, the output or the product or even the by-products and also their respective process conditions or say the overall process condition. Now for that, we need to understand, what are the process variables? And what are typically those parameters?

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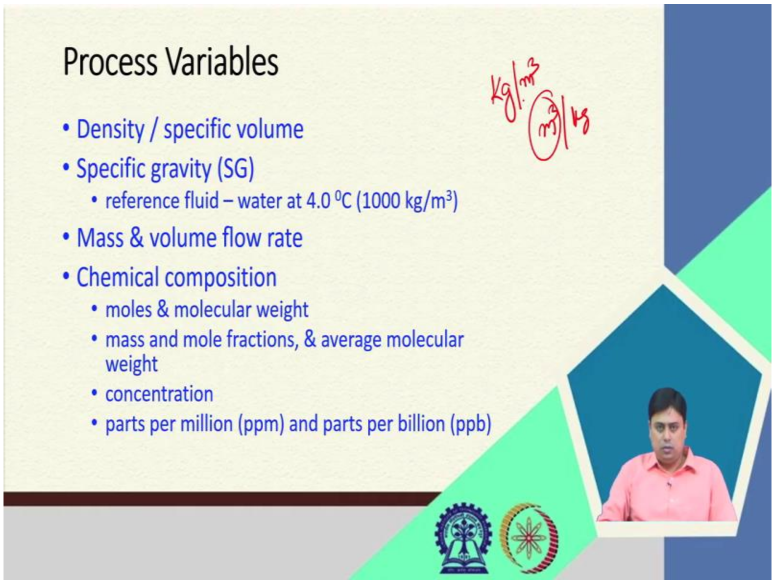

Process Variables

- Density / specific volume
- Specific gravity (SG)
  - reference fluid – water at 4.0 ^{0}C (1000 kg/m^3)
- Mass & volume flow rate
- Chemical composition
  - moles & molecular weight
  - mass and mole fractions, & average molecular weight
  - concentration
  - parts per million (ppm) and parts per billion (ppb)

Kg/m^3

$\boxed{m^3}$/kg

So, the typical say the material properties in fact are the process parameters. So, for example, we know that the mass, volume, density, specific gravity, mass and volume flow rate, etc., the pressure, system pressure and its concentration, etc. So today we will focus on a couple of the more relevant one that is essential for our course and others I understand and I believe that we were quite aware of those things.

In fact, all these points you are aware of it is just to refresh your memory. So we know the density how it is defined, it is mass per unit volume. Sometimes the density is also defined, or it is also mentioned by the specific volume, which is the inverse of density that is, we have the amount of a substance or a species, it is the volume of the species per unit mass of that substance. That is the density as a unit of kg/m^3 in SI, so in specific volume, we have m^3/kg that means the substance volume that it occupies for its unit, mass. That is the specific volume.

The density and the specific volume sometimes used are interchangeably. Now we have also understood the term called specific gravity. Specific gravity is basically the ratio of the density of the property and a reference fluid. In most cases, and if it is not specifically mentioned, the reference fluid is typically the water at 4°C, when we consider its density, typically the water density is 1000 kg/m^3.

So, which means specific gravity of 0.5 of any species or component means its density is 500

kg/m^3. So, such kind of say process parameter or the process term would be given in a problem statement or the design statement which you need to understand and convert during the calculation. We also are aware of the flow rate, and that can be either the mass flow rate or the volumetric flow rate.

So mass flow rate is the unit of say when we have kg/s. The volumetric flow rate is basically say, m^3/s. Which is the amount of mass that is fed or that is being flown per unit time similarly it applies for the volumetric flow rate as well as the amount of the volume that is flowing per unit time. So this mass and volume flow rate, this conversion can be done using the density term, because we know the relation between the mass, volume and the density.

So, for such simple things were not going into the details because it is understood that you are already aware of those things. It is just to tell you that such kind of conversions we will encounter in future and we should be aware of this conversion that if the mass flow rate is given and the density of the species is known we should be able to convert that to the volumetric flow rate or the vice versa.

Now the other important one is the chemical composition. The chemical composition includes, say, the chemical composition understanding includes say the number of moles of the molecular weight of the substance, mass and mole fractions or the average molecular weight or the concentration of the species. And here in the concentration of the species to a specific unit, we will understand those are the PPM and PPB that is the parts per million and parts per billion.

These are used frequently when there is the solute is in trace amount that means it is the very minimum amount. That if you try to express that in terms of grams per unit volume or say the whole substance, that value would be very, very lower, a very minimum value. So then this kind of units comes into play which helps us to understand the number in a better way. So the moles again this thing we are aware of. What is a mole? What is molecular weight? What is mass and mole fraction?

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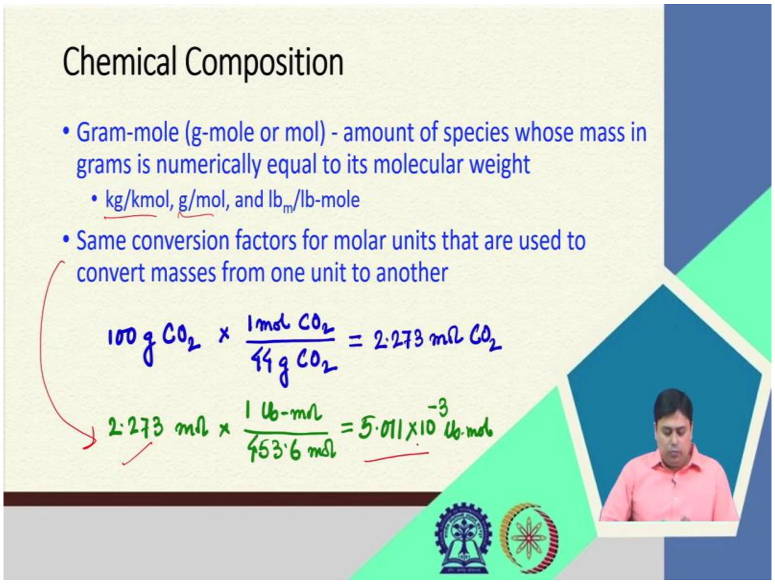

Chemical Composition

- Gram-mole (g-mole or mol) - amount of species whose mass in grams is numerically equal to its molecular weight
  - kg/kmol, g/mol, and lb_m/lb-mole
- Same conversion factors for molar units that are used to convert masses from one unit to another

$$100\ g\ CO_2 \times \frac{1\ mol\ CO_2}{44\ g\ CO_2} = 2.273\ mol\ CO_2$$

$$2.273\ mol \times \frac{1\ lb\text{-}mol}{453.6\ mol} = 5.011 \times 10^{-3}\ lb\text{-}mol$$

How do we calculate the average molecular weight? How do we define concentration? So here let us start with the concept of mole. So typically, we express that in gram mole or simply mole which is the amount of the species whose mass in grams is numerically equal to its molecular weight, and that is typically expressed by such unit that is kg/kmol, g/mol which we mention it simply also expressed as more if it is mentioned as a mole that means it is a g/mol and pound mass per pound mole in the different unit system.

So now the point is that these molar units when we try to convert say we are given with a g/mol, and we have to convert that unit for our calculation since the unit consistency is necessary. So we have to convert that to pound mass per pound mole such unit. Now in these cases, the conversion factor remains the same, which is used to convert the masses for that respective conversion.

Say for example from gram to pound-mass, whatever the conversion factor is that itself can be used in order to convert these molar units. So we will see an example. Say we have 100 grams of CO_2, now our job is to calculate that how much mole of CO_2 is here. This is a very simple task. So in this case what we do, We calculate the molecular weight of carbon dioxide which is 44 that means we have 44 g of CO_2 in this 1 mole of CO_2.

So that means 100 grams of CO_2 is basically 2.273 moles of CO_2, this is how we convert from the mass to the molar composition with the help of molecular weight. Now if we have to convert this gram mole to pound mole. Now, this is the stage that I mentioned earlier that we typically understand or know that 1 pound is basically 453.6 grams, so 1 pound-mass is 453.6 grams. So, the same conversion factor, we can use to convert the gram mole to the pound mole.

And in this case, we convert it like this and we get this final value. Now here let me reconnect with my previous lecture on the significant figures. So, here you see the calculations that are done here in this second Stage particularly. It is showing the example of how significant figures how many significant figures have to write and how to round it off. So here specifically, it should have been written as 100.0 grams. Then what would happen then what you have is basically here you have 4 significant digits and that is why it is expressed as the final result in 4 significant figures.

In this case, also we have the minimum number that is the four significant figures, and it is expressed in such a way. So in future, I may be omitting this things but this is the thing that we should ideally follow. So now this is the example that I gave you for the conversion of gram mole to pound mole.

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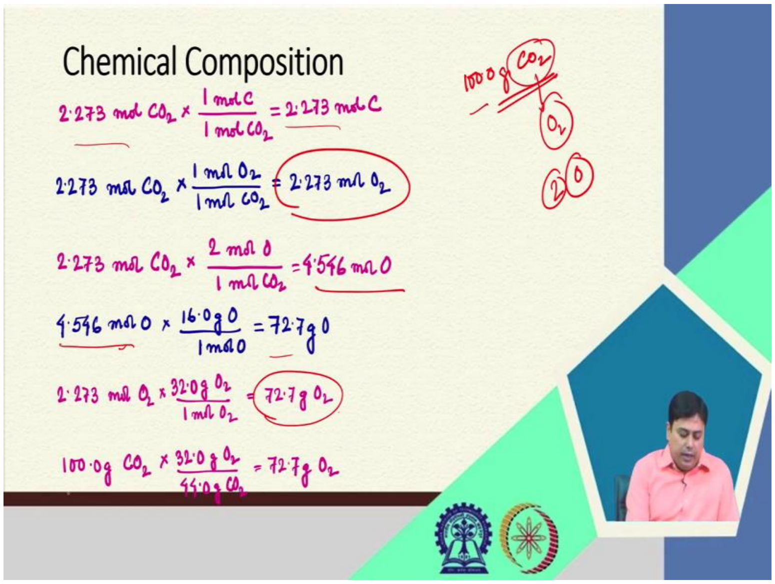

Chemical Composition

$$2.273 \text{ mol } CO_2 \times \frac{1 \text{ mol } C}{1 \text{ mol } CO_2} = 2.273 \text{ mol } C$$

$$2.273 \text{ mol } CO_2 \times \frac{1 \text{ mol } O_2}{1 \text{ mol } CO_2} = \boxed{2.273 \text{ mol } O_2}$$

$$2.273 \text{ mol } CO_2 \times \frac{2 \text{ mol } O}{1 \text{ mol } CO_2} = 4.546 \text{ mol } O$$

$$4.546 \text{ mol } O \times \frac{16.0 \text{ g } O}{1 \text{ mol } O} = 72.7 \text{ g } O$$

$$2.273 \text{ mol } O_2 \times \frac{32.0 \text{ g } O_2}{1 \text{ mol } O_2} = \boxed{72.7 \text{ g } O_2}$$

$$100.0 \text{ g } CO_2 \times \frac{32.0 \text{ g } O_2}{44.0 \text{ g } CO_2} = 72.7 \text{ g } O_2$$

Now along with that, say in these 100 grams of CO_2 how many moles of carbon, oxygen, atomic oxygen, and Molecular oxygen is there? This also we can have the results from this understanding. So we have seen that 100 grams in this, here we have seen the 100 grams of CO_2

means 2.273 moles of CO_2. Now in that mole of CO_2, we basically have the same mole of carbon, because we see that in 1 mole of CO_2 we have 1 mole of carbon.

In 1 mole of CO_2, we also have 1 mole of O_2 the molecular oxygen. But in 1 mole of CO_2, we have 2 moles of atomic oxygen. So, the number of mole per atomic oxygen is 4.546 mole O. So for any compound we can individually identify the species and we can find out its detailed composition. Now the point is that if we try to come from molar composition to the weight or the mass composition. The similar process we may follow is that this much mole of O, the atomic oxygen means 72.7 grams of atomic oxygen.

Because 1 mole of atomic oxygen means 16 g of O, with that conversion we convert molar composition to the mass composition. Similarly, we have here this much mole of molecular oxygen which means we have this much amount of molecular oxygen because 1 mole of O_2 is basically 32 grams of O_2. So that means in 100 grams of CO_2 we have 72.7 grams of O_2. Now, this also can be calculated.

The other method or the different way is that 100 g of CO_2 and here in 1 mole of CO_2 we have 44 g of CO_2, where we have 32 g of O_2. So that means in 100 g of CO_2 we will have 72.7 g of O_2, which is kind of an identical answer that we can get the other way. Now here in these, all calculations see since this is the initial period and in the module itself, we have understood the importance of significant figures of the significant digits.

Here all the calculations are consistent in that respect. So, for example, in the last one, we have here, the minimum significant digits is 3, so the final result is rounded off to 3 significant figures. But the aim of this slide is to have you understood that how we convert molar composition to mass composition and how we find out individual species composition in a compound.

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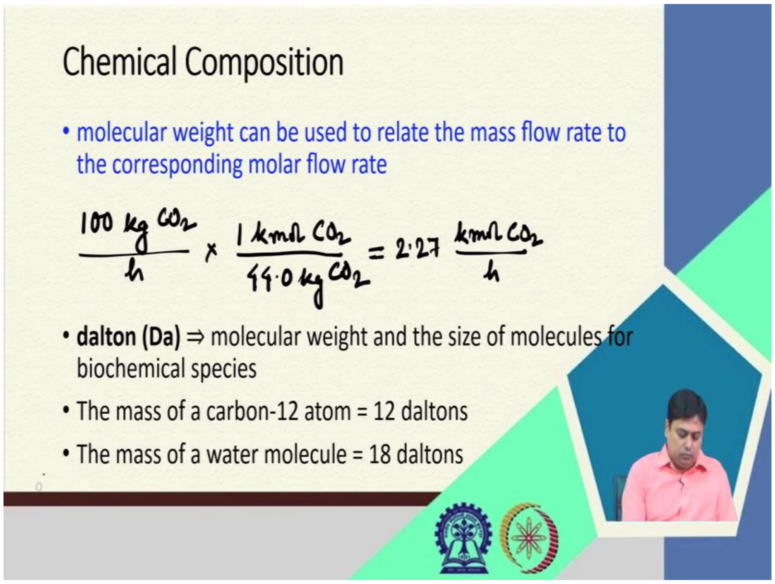

Chemical Composition

- molecular weight can be used to relate the mass flow rate to the corresponding molar flow rate

$$\frac{100\ kg\ CO_2}{h} \times \frac{1\ kmol\ CO_2}{44.0\ kg\ CO_2} = 2.27\ \frac{kmol\ CO_2}{h}$$

- **dalton (Da)** ⇒ molecular weight and the size of molecules for biochemical species
- The mass of a carbon-12 atom = 12 daltons
- The mass of a water molecule = 18 daltons

This molecular weight can also be used to relate the mass flow rate to the corresponding molar flow rate because eventually, we can convert the mass composition to the molar composition based on molecular weight. And similarly this mass flow rate can be converted to a molar flow rate. So for example, if this 100 kg of CO_2 is flowing in an hour, which means the flow rate of the CO_2 stream here now say I introduce the term process stream that contains 100 kg of CO_2 per hour.

This we can convert with the help of its molecular weight to say the molar flow rate. And the unit of the molar flow rate is consistent with our previous understanding that is the kilo mole of CO_2 per hour. Similarly, we can do it for a different style of the units. Now one term some may encounter is the dalton. The dalton also represents the molecular weight and the size of molecules for several biochemical species.

The definition of dalton is the weight of that species with reference to the C 12 atom. So, 1/12th of the C 12 atom which means the mass of a C 12 atom is 12 daltons and the mass of a water molecule is 18 daltons. So this term also you may encounter and that is why we have introduced it here for your understanding.

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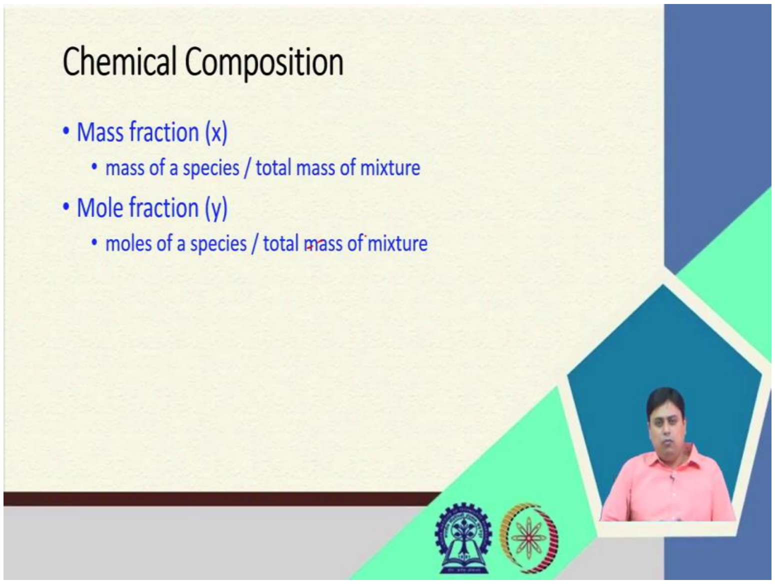

Chemical Composition

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

Now we go to the mass and the mole fractions. So If we know this fraction, the mole and the mass fraction, these concepts are pretty useful and it is necessary when we have a mixture of species or individual species. We have a mixture of CO_2, O_2, nitrogen these gases. Then if you know the individual masses of these species, we can calculate the mass fraction easily. This concept we are aware of how to calculate the mass fraction.

And also, we should be able to calculate the mole fraction in the sufficient information is given, that means mass and mole fractions are basically the amount of the species, the mass of the species or the total mass of the mixture. And similarly, if we have the mole fraction, it is the moles of the species with the total moles of here. It would be the total moles of the mixture. That is the total mole fraction that is the mole fraction of individual species.

So will continue from here in the next lecture, and we will see how do we convert the information, mass fraction and the mole fractions and we interchange any whether we can use it and how to use it. So with this, I stop here today and will see you in the next lecture. Thank you.