Material and Energy Balance Computations
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Lecture –28
Single Phase Systems

Hello, everyone, Welcome back once again in the NPETL online certification course on material and energy balance computations. We are. Now on a different module than that we did in the last week. So, in this next 3 classes what we will see that in the last couple of problems or in fact, all the problems that we have seen, you have realized that all the properties, all the material properties the species or the components were conveniently given.

But in most of the scenario what happens that you do not have those information's readily available in the problem statement and that is frequently encountered when we handle single or the multiphase systems. So, in these next 3 lectures, I will briefly introduce a couple of important terms that will be picked up in the next module that will start on the energy balances. Now for that this is you can consider as the foundation and learning a few key terms.

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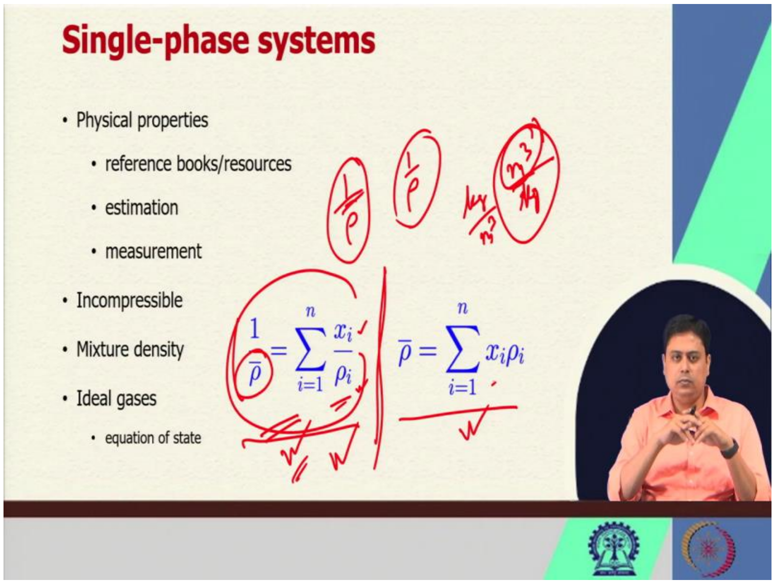

Single-phase systems

- Physical properties
  - reference books/resources
  - estimation
  - measurement
- Incompressible
- Mixture density
- Ideal gases
  - equation of state

$$\frac{1}{\bar{\rho}} = \sum_{i=1}^{n} \frac{x_i}{\rho_i} \qquad \bar{\rho} = \sum_{i=1}^{n} x_i \rho_i$$

$\frac{1}{\rho}$ $\frac{1}{\rho}$ kg/m^3 m^3/kg

So, in the case of a single phase system although in practice whenever we deal with an industrial material balance problem, those are of multiphase in nature let us begin with the single phase system. Now as I mentioned, the physical properties that you have seen in those last few problem statements or whatever we have done till now I have given all the information or typically the problem statement consisted all the necessary information regarding the properties of these species.

Now these physical properties are not readily available in the problem statement, in most of the cases. So, for that, what you have to typically do when you actually will solve the design problem or you apply this knowledge in somewhere else is you may have to refer some reference book or the resources for those physical properties for example, the density, different volume at different temperatures and pressures.

So, you have to consider these references, books and one of the main resources of these physical properties is the Perry’s handbook, there are several handbooks as well. The other way that we can do or we can obtain these physical properties are by estimation that is, we estimate the physical properties based on some given correlations by the previous researcher or previous scholars. So, they typically have say, performed a set of experiments in order to find out those physical properties.

But your desired physical property is not falling in the range of their studies operating conditions. So, in those cases what we typically do that we typically estimate from those correlations. Now when those correlations are derived based on several experiments we typically call those as empirical relations. Several correlations have been suggested because see it is very difficult or it is very impractical that whenever we deal with a reactant to form the product, the reactant would be of pure in nature.

And if the pure substance is not there, if there are impurities at certain percentages of their which are saying inert or impure then what happens the physical properties of the pure substance cannot be directly put into the system or during the calculations for the sake of simplicity we can do that, do that, but for accurate calculations you may have to counter or you may have to take into account those impurities or those mixture cases.

So, in those cases we have to calculate, say a mixture density or say different other properties of the mixture. Now those are given by previous researchers in a wide set of correlations, we have to pick one and we have to use that appropriately. The other way or the most accurate way would be to measure that directly experimentally, which is which is typically very difficult in several cases. If we can do that, that is the best way we can have it the measured physical properties, but these experiments are cumbersome.

These are difficult to do in certain cases and also expensive time consuming. So, these are the ways that where we can find the physical properties of the material if those are not given in the problem statement. Typically, that is why if you pick a text book on these subjects. You would see that the appendix there is a lot of lots of tables are there, lots of data out there base for these physical properties, if you if you pick a heat transfer book, you will find the thermal conductivity values all the material properties values.

So, similarly, if you pick up this chemical material balance book you would find there are several properties that are given at different temperature pressures etc. So, then there is a term. So, what happens, say you have gas, liquid and the solids that these 3 substances you are handling. Now say you are changing the pressure temperature of the system. Say something comes into the reactor at a certain temperature and pressure, and goes out of the reactor but at different temperature and pressure, and if that substantially varies.

Those 2 are substantially different then the gaseous product its properties are more likely to change than the solid and the liquids. So, when this density change does not occur with the variation of pressure or say we neglect that we consider that time that these substances are incompressible in nature. If the density varies with the pressure we considered that as the compressible substance.

So, these are the things kind of adjectives you would find in the problem statement, and then you can simplify the problem statement by considering that density is not varying for that substance if you find the term incompressible. Then the point that I was mentioning that say now instead of a pure substance you have a mixture of several species that are fed into a reactor or into some process, the system.

So, in those cases, we have to find the mixture density and how do we find mixture density? There are 2 ways we can find the mixture density. One of the ways is this expression where this ρ bar is the mixture density or we say the mean density of that mixture. Now this is equals to. So, this is one by this density term that we have it is basically the summation of n number of species where i is the counter of the species x is the fraction, the mass fraction of that the species in the mixture and this is their pure substance density of that, i^{th} component.

We add these things up for n number of pure substance, and we get this density the mean density of the mixture through this expression. So, here the point is that one-one assumptions, inherent assumptions that we have made here, which we call the additive nature of the volume that means you take 2ml of certain substance or say, component A, you add this with 1ml of substance B you get 3ml of the product which is substance C.

If this happens, then we can find out this, mean density or the mixture density through this way. Now the point is that with this assumption we apply this expression that the volume additivity is there for that problem. The other way of finding this mixture density is using this expression which is the average of the pure component densities. So, here we just add these mass fractions multiplied by the pure component density, and we take an average of this.

This averaging is happening based on the mass fraction of that material. Now here, the density we are calculating as an inverse of that term. So, in this case, whenever we considered such scenario or 1 / ρ, we typically call this time as a specific volume, the specific volume, if it is ρ bar, it is the specific volume of the mixture, or it is a specific volume of the substance, because see density is in a SI kg/m^3.

Inverse of this is m^3/kg. So, that is why it is the inverse of the density is a specific volume because you have this much of a volume per unit mass of the substance it is the measure of the amount of the volume per unit mass of that substance. So, sometimes you would be given with the specific volume information. So, do not forget to convert back to the density value or the mixture density, whatever it applies.

Now, the question is that which one we will use if there are 2 relations by which we can find the mixture density, which one is a more accurate. The point is as I mentioned, that inherent assumptions here that if the system does not go with the volume additive in the nature then naturally, we use this expression. But when both are applicable in that case, we typically calculate both of these and then we try to find out the deviation of this value if there is any reference substance density or say any experimental value.

Now if there is an experimental value then why there would be necessity of doing this thing? The reason is that this acts as a validation point that this calculation is being applied for that reference substance or that kind of substance which we will use after validating to similar type of the substance that is in nature in structure or in formula. So, as a thumb rule, it has been seen or as a thumb rule, it can be said that this specific volume formula quite well, agrees when you have similar type of the substance that you are mixing.

So, for example when you have, so, this this is a kind of similar substances of having equivalent molecular weight we can put it in this way instead of similar substance. So, for example if there is a straight chain hydrocarbons that are mixed. So, the straight chain hydrocarbons for examples, you have normal pentane, normal hexane, normal heptane these mixtures when you mix and try to find out you mix in a different proportions and then you try to find out its mixture density, then this expression applies or predicts the mixture density or estimates mixture density in a reasonably accurate way than the other one.

But there is no as such hard and fast rule that which one should be applied and the other one should not, but I told you the inherent assumptions of this expression because based on that assumption, this equation can be derived. So, that means we now can calculate the mixture density if we know the mass fraction of the pure substance and the pure substance densities. Now this is the point once again that the pure substance densities there are thousands of such compounds or materials are available, and for all of them the values are typically we do not have readily available.

So, we look at the reference book or the reference resources or sometimes we estimate those from the standard correlations that are given. Then the term you possibly have heard and you know what is ideal gas? We will not go into the definition. I just will try to make you remember this thing that in ideal gas this is important because this ideal gas we know immediately, it comes to our mind that there is an expression $PV = nRT$ the ideal gas equation.

Now that means what it does those equations, those equations are typically called the equation of state. This equation of state is basically gives us the relation between the molar volume and the temperature and pressure. So, if you remember this term that , if you go to the term, P, V, n, R, T. So, V is the volume, n is the number of number of moles, P is the absolute pressure, T is the absolute temperature, R is the gas constant.

So, that means it gives us the relation between the molar volume or the molar quantity the volume the temperature and pressure. So, for any gaseous substance that I mentioned that it immediately changes its volume due to its different state, which is the temperature pressure if we assume the ideal gas equation of state applies in those cases or this the mixture of the gaseous mixture behaves as ideal gas.

Then we can quickly what would be its volume at the desired temperature and pressure if we know at a reference temperature and pressure the volume.

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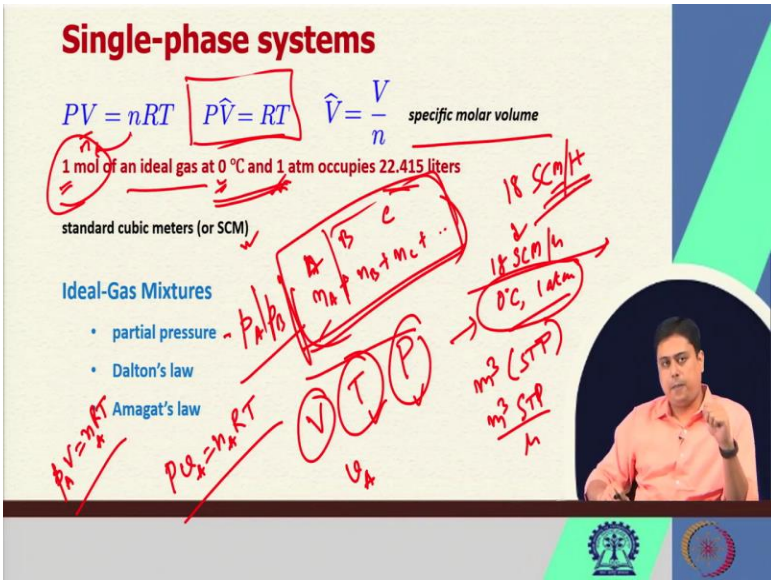

Single-phase systems

$PV = nRT$ $\quad P\hat{V} = RT \quad \hat{V} = \frac{V}{n}$ specific molar volume

1 mol of an ideal gas at 0 °C and 1 atm occupies 22.415 liters

standard cubic meters (or SCM)

Ideal-Gas Mixtures

- partial pressure
- Dalton's law
- Amagat's law

Now these R gas constant, the PV = nRT here, the R is the gas constant you know, the value and the value changes according to the units that we use for the pressure and temperature, as well as the value of V, because this unit becomes PV / nT. According to your choice of the unit system SI, C.G.S., or FPS you would have different values of this universal gas constant the numerical value changes.

Sometimes it is difficult for you to remember that all the things, all those numbers. Now the point is that expression that PV is equal to nRT we can further write it this way in terms of the V hat, where this V hat that we have is called the specific molar volume. So, this is called specific molar volume. So, it is just V / n here and then we have the similar expression, the same expression written a different way.

Again, remember, P here is the absolute pressure you should be able to differentiate between the absolute pressure, atmospheric pressure and gauge pressure and the relation in all the three. T is the absolute temperature. So, now we also know that one mole of I mean, based on this expression, if you if you place this temperature and pressure and the universal gas constant we see that one mole of ideal gas be it any gas irrespective of gas component.

If it behaves as ideal gas, then then that will occupy this 22.4 litres and that is for 1 mole of that gas species or the gas mixture. So, 1 mole of an ideal gas at 0°C and 1 atm occupies 22.4 litres.

So, this thing you must remember because this helps in conversion in the problem statement, because there we frequently been encounter, this change in pressure and temperature from the inlet to the outlet or say when 2 different streams are mixed at a different temperature and pressure, and we have to estimate basically in terms of moles.

The term standard cubic meters or the SCM or SCF when there is the FCS unit that is the standard cubic feet. Now this is SCM or the SCF this standard refers to this standard temperature and pressure that this is a reference temperature and pressure where we find for example, here that I mentioned that the reference temperature in this case was zero degrees centigrade and one atmosphere, and there we have seen that if n is one mole, it is basically 22.4 litre as the V the volume.

So, this condition, usually the standard temperature and pressure it usually refers to the zero degree centigrade and 1 atmospheric pressure and the volume at that temperature and pressure is typically referred as standard cubic meters. So, in the problem statement, you would see that this gas is flowing at say 18 SCMH, which means standard cubic meter per hour. Now if that is mentioned then in that stream, while labelling the flow chart, you must write that it is 18 SCM per hour at zero degrees centigrade and one atmosphere.

Because this now, will not be explicitly mentioned because it is already mentioned as the standard cubic meter per hour. So, this standard cubic meter per hour is typically also sometimes mentioned as meter cube STP or say simply meter cube STP per hour. So, the point here that if we say this 18 standard cubic meter per hour it means that this is flowing at zero degrees centigrade and one atmosphere and this 18 meter cube per hour of the gas streams.

Now when nothing is mentioned about the reference temperature and pressure there, we use this inherent values or default values if it is explicitly mentioned that the reference temperature and pressure is different than that, you must write that in the flow chart or during the calculation, you have to take into account. Now coming to the point that as I mentioned hardly we deal with any pure component in practical case.

So, what we have like the mixture density that we calculated for the liquids. Here there are several things that you have to understand and will be required in the energy balances is the ideal gas mixture and there, what is the term called partial pressure. So, the partial pressure is basically says, you have a substance A, you have another substance B or C the species that are mixed in such a way that $n_A + n_B + n_C +$ etc, these are the mixtures of component A or species B, species C etc.

Now this is contained in a volume which is capital V at a temperature capital T and the total pressure of this vessel or the enclosure where all these mixture are there, say, is capital P. So, the partial pressure of any component be it P_A, P_B or P_C or the other components is the pressure that that component would have exerted if only pure substance were there in that volume and at that temperature.

So, which means as if there is no other parameters or other substances in the same enclosure without changing the temperature and keeping the volume constant the amount of pressure it would exert alone in absence of any other species that pressure would be called the partial pressure of that component and we typically designate by small p and the subs subscript A. So similarly, p_A, p_B, etc, would be the partial pressures of the component A, B, C, etc.

And say in a different note. Now say you have this standard temperature and pressure fixed of that vessel, the total pressure and temperature you kept it same of that container. But you allow the volume to change then the amount or the volume that would it acquire a certain species that is pure substance in A in such case that is a small v_A that is the volume that the component A would occupy at this temperature and this pressure if it were there alone as a pure component.

So the point is that when these individual species behaves as ideal gas then also, we can write it for it that capital P small $v_A = n_A$ RT or when the partial pressure is involved. So, in that case, we can write n_A RT, $p_A V = n_A RT$.

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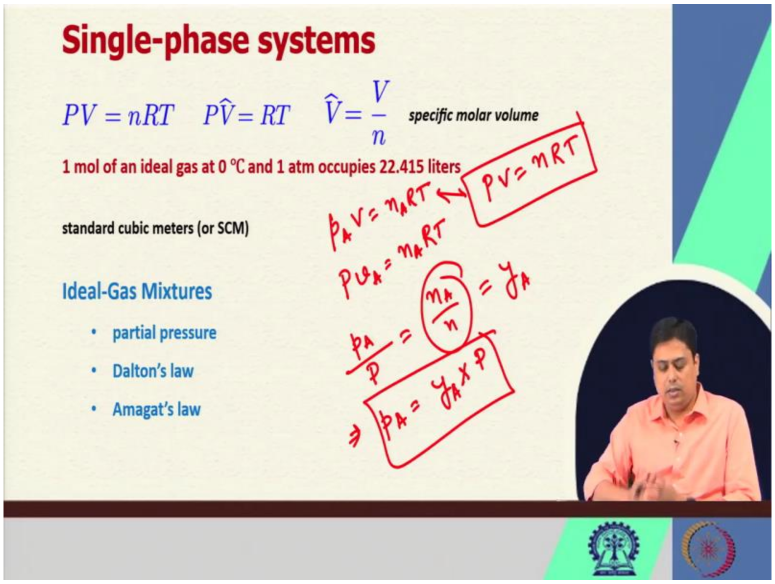

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- Amagat's law

$\boxed{PV = nRT}$

$p_A V = n_A RT$

$P v_A = n_A RT$

$\frac{p_A}{P} = \frac{n_A}{n} = y_A$

$\Rightarrow \boxed{p_A = y_A \times P}$

Now this thing so, if this as I mentioned, if this behaves individually as ideal gas and also if it is like in both the cases and we have PV = nRT, the whole mixture is also behaving as ideal gas. Then if we divide this and this relation, so, the first one divided by the second one, what we have is this relation. Now this is the mole fraction of component A which we say that this is y_A that means the partial pressure of component A is the mole fraction × the total pressure that is, the partial pressure of a substance or a component in an ideal gas mixture is that the mole fraction of that component × the total pressure.

This is how you can calculate the partial pressure of that component. I hope till this point, it is very clear to you I will pick it up from here in the next lecture. And we will go on explaining that what are these Dalton's law and Amagat's law how that is useful to remember till then, thank you for your attention.