Mass, Momentum and Energy Balances in Engineering Analysis
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Lecture - 13
Material Balance Involving Chemical Reactions

Welcome. After learning about the techniques to handle the various reactions, how to find the conversion, how to find the extent of reaction the yield from a reaction etcetera, now what we shall do in this lecture we shall be using those concepts in carrying out the material balance. You may recall before this lecture, we have done the material balances without any generation or consumption term and that was because none of those systems had any kind of reaction terms involved. Now, what we are going to do in this lecture is that we are going to involve the reaction terms, so that the generation or the consumption terms in the mass balance will not be nullified.

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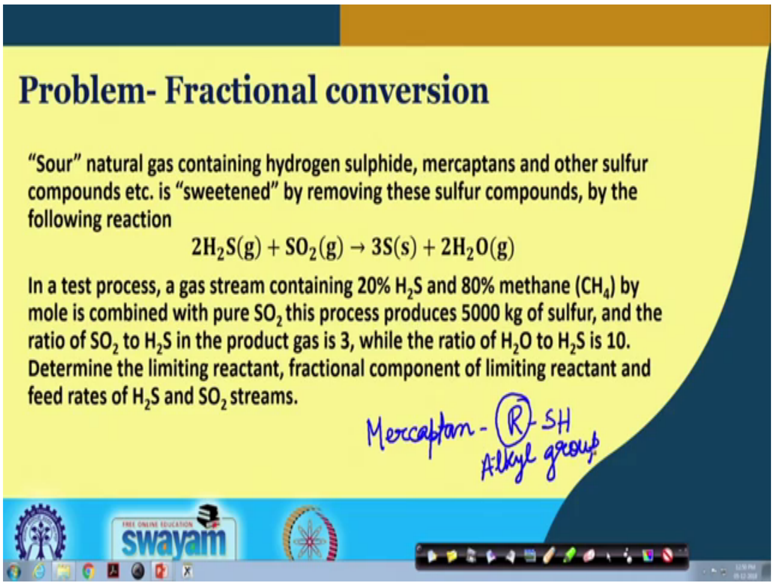

So, first we take up a problem like this, that we have a sour natural gas that contains hydrogen sulphide, mercaptans and other sulphur compounds. Now, what happens that whenever we are getting the natural gas from the earth it has main impurities and that is why the raw natural gas cannot be used directly for our consumption. So, what we do we, take out all the impurities and one of the impurities is sulphur and its compound.

So, we have the hydrogen sulphide which needs to be removed, because if it reacts with water it forms mild acids and because of this the pipelines or the equipment through which the raw natural gas passes would get corroded. So, we need to take out this particular gas, and not only that other sulphur compounds like mercaptans. And what are mercaptans? Mercaptans are compounds of sulphur which are hydrocarbon in nature, the general formulation of mercaptans is like this R-SH. Now, this R is some kind of an alkyl group.

So, we have various types of mercaptans which gives some kind of foul odour to the particular compound. And even though mercaptans are undesirable in case of natural gas, but we do use the mercaptans also as an indicator of the gas leakage especially at our household LPG cylinder. So, whenever there is some kind of leakage in the LPG cylinders at our kitchen, we smell some odour and that is due to this particular compound mercaptans ok. So, but in case of raw natural gas, it is a waste product, and this has to be removed.

So, what we have that these particular natural gas when we are removing the sulphur compounds, we have what we call sweetened natural gas. So, raw natural gas with the sulphur compounds is called sour natural gas. And the when the sulphur compounds out, we have sweetened natural gas or sweet natural gas not by test, but the by the presence or absence of the sulphur we are making this sour and sweet nomenclatures.

Now, one way of removing this H 2 S is that we react it with SO 2 that is sulphur dioxide, so that we get the sulphur in the solid form and we get water vapour. So, here you see this is the reaction in which we have the H 2 S and SO 2 in gaseous form, and sulphur in solid form, and water in gaseous form again. So, in one of the tests of such kind of reaction a gas stream containing 20 percent H 2 S and 80 percent methane by mole is combined with pure SO 2.

Now, you see that why methane because natural gas is primarily methane. So, what we are doing that in such some particular test in the laboratory, the methane was taken along with that we are putting the H 2 S in is as impurity. And this process produces 5000 kg of sulphur and the ratio of sulphur dioxide to hydrogen sulphide in the product gas is coming to be 3, while the ratio of the water vapour to H 2 S is coming to 10. So, we have to determine the limiting reactant the fractional component of limiting reactant and feed rates of H 2 S and SO 2 streams.

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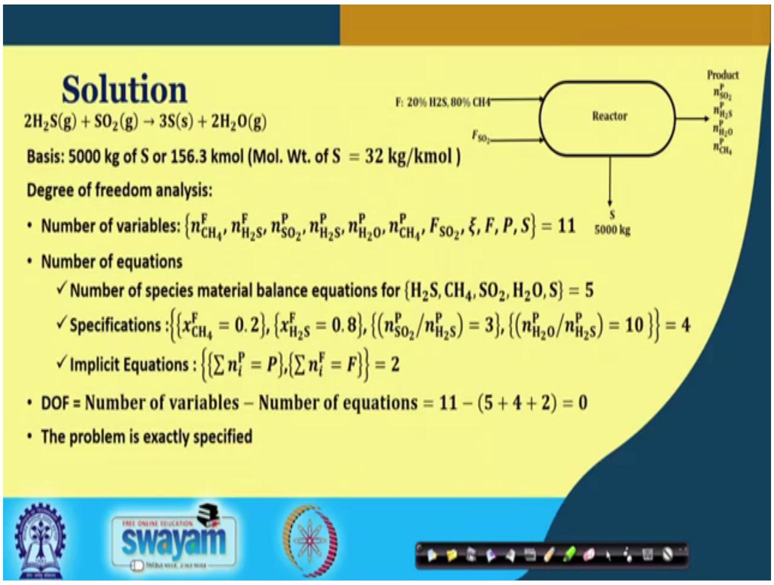

Now, for this what we do this is what we have now see that reactor here. Now, in the reactor we are putting all kinds of the raw materials, we have the methane over here and H 2 S plus SO 2, we are feeding. And this SO 2 is going to react with H 2 S and the methane will come out without any kind of reaction. So, on this product side, we have methane plus H 2 S, SO 2 and H 2 O. So, this we find as some amount of unreacted H 2 S is also coming out of the reaction. And here we have shown separately the solid sulphur.

So, after writing the reaction, what we do we have the basis as 5000 kg of sulphur or we convert this into mole because all the reaction calculations are done based on the mole as we have learned in our earlier lecture. So, we know that the molecular weight of sulphur is 32 kg per kilo mole. So, we simply divide this 5000 kg by this 32 kg per kilo mole, and we get these many moles of sulphur as sulphur

Now, before we go onto do further calculation in any kind of problems we do we apply the degrees of freedom. Now, this degree of freedom tells us whether we have enough number of equations to solve for the various numbers of unknown variables. And about degrees of freedom I have told you in my earlier lecture. So, initially whenever you are doing such kind of problems, it is advisable that you go through this degrees of freedom analysis and as you gain expertise, then perhaps you may not do this particular step in solving your problem.

So, let us first see that how to do this degrees of analysis degrees of freedom analysis. So, here we have the first we count the number of variables involved in this particular system. So, we have all the number of moles of the various species over here in the feed and in the product. So, this F superscript represents the feed, and the P superscript represents product, and this F SO_2 is the amount of SO_2 going in the feed stream. This is the extent of conversion, and this is the or vertical fractional conversion. And this F, P, S are the flow rates of the feed, the product for the gases and S is the for the sulphur ok.

Now, please do not confuse this S with this sulphur. This is just a representation of the solid; this S stand for solid not for sulphur. So, if you count all these variables, it comes out to 11. Now, after this we need to know how many independent equations we can get to solve for all of these variables. So, here you can see that we have first we apply the material balance, and we find that for each of the species we can write a material balance. So, we identify these species. So, we have five species. So, for each of them, we can write one material balance, so that will give us five number of material balance equations.

Then some of these things had been specified in our problem. So, those will also be counted in this number of equations. So, these are the specifications given in the problem. So, we put them here and we get this count to 4. And then we have some implicit equations that is those equations which have to be obeyed. Like for example, summation equations, as I told you in my earlier lecture that the total amount of the species in a given stream should give us the total amount of the particular stream. So, here we find if we sum up all the number of moles in the product, we should get the total product amount. Similarly, we can do it for the feed side. And so these two equations are called summation equations. So, in these two summations equations give us two mole equations.

So, now what we do we simply count all these numbers. So, we get 5 plus 4 plus 2 that means 11. So, the degrees of freedom is number of variables we have 11 minus number of equations also 11, so that is gives us 0. Zero means that the problem is exactly specified that means whatever may be the unknowns we have, rest of the variables out of these variables whatever we know and whatever rest are remaining all of them can be determined by the given set of data.

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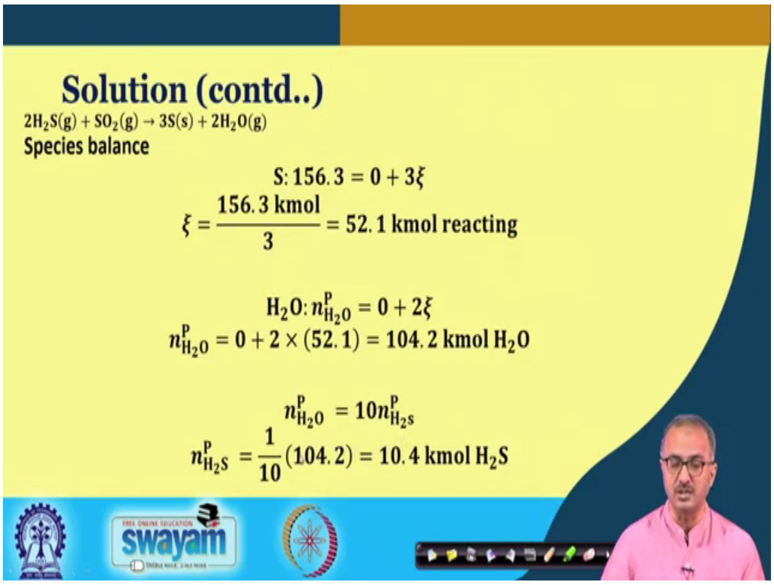

Now, let us do species balance one by one. First let us look at sulphur. Now, from the definition of the extent of the reaction, we put this thing and we get the extent of reaction as this 52.1 kilo mole reacting. Once we know this zeta value, now we do one by one for the other components like H 2 O. We find the in the product stream, we will be having with this particular equation these many moles of the H 2 O. Next we go to this amount of H 2 S, when we can see from the stoichiometry that the number of moles of H 2 O is 10 times the number of moles of the H 2 S. So, we get the H 2 S amount like this from the number of moles of water.

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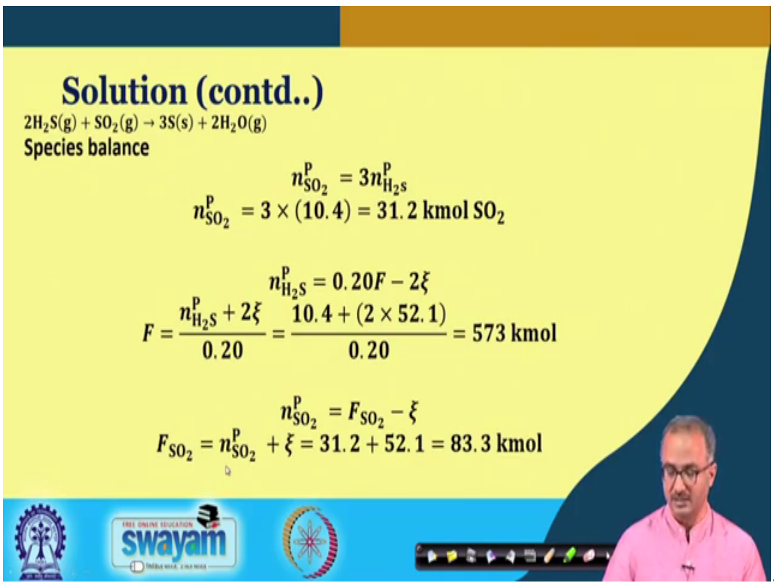

Next we go to sulphur dioxide. Again we go to the (Refer Time: 10:41) with the stoichiometry. And we see that the sulphur dioxide will be 3 times that that of the number of moles of H 2 S. So, here we get the amount of sulphur dioxide. Then we come to the H 2 S. And here for the H 2 S we write for this because we know that how much H 2 S is present in the feed. So, we write the 20 percent is there. So, 0.2 into F and from that we find out the amount of feed. And then similarly we go to the product side and we have seen that how the product and feeds are related. So, we find this particular thing this n P SO 2 equal to F SO 2 minus zeta from the definition of zeta, and we find this is the amount of the a SO 2 in the feed stream.

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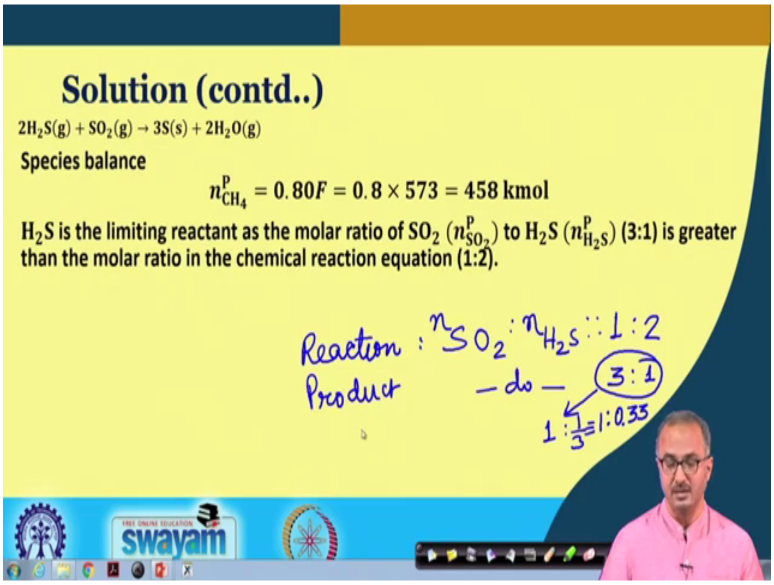

So, similarly we apply it for the methane. And we see this is the amount of methane. And this methane we see that it is coming unreacted. So, whatever methane is going into the system is also coming out of the reactor. So, we find the amount of methane in the product and the feed stream are the same. Now, after doing all this calculations for the various mole fractions and the feed rates and product rates, now what we have to do that we have to figure out which is the limiting reactant.

Now, as per the stoichiometry, if you look at the stoichiometry of the reaction, you see that we have been given that for two moles of H 2 S will react with one mole of SO 2. And here we are given that in the product what we have 3 moles of SO 2 per mole of H 2 S. So, what we find? So, if we write like this, if we write like this that for the reaction the reaction what we see the SO 2 amount or rather n SO 2 is 2 n H 2 S is how much it is 1 is to 2 ok. But, on the other end in the product what we find that same ratio is given as 3 is to 1. And this may be reduced like 1 is to 1 by 3 that is same as 1 is to point about 0.33 ok.

So, now what we find that for reacting this 1 mole of SO 2, we need at least two moles of H 2 S by stoichiometry, but what we find that in the product we do not have so much we have only 0.33 mole that means, in this case we find that the H 2 S is the limiting reactant and not SO 2. So, this is how you can find out the amount of the or the identify the limiting reactant.

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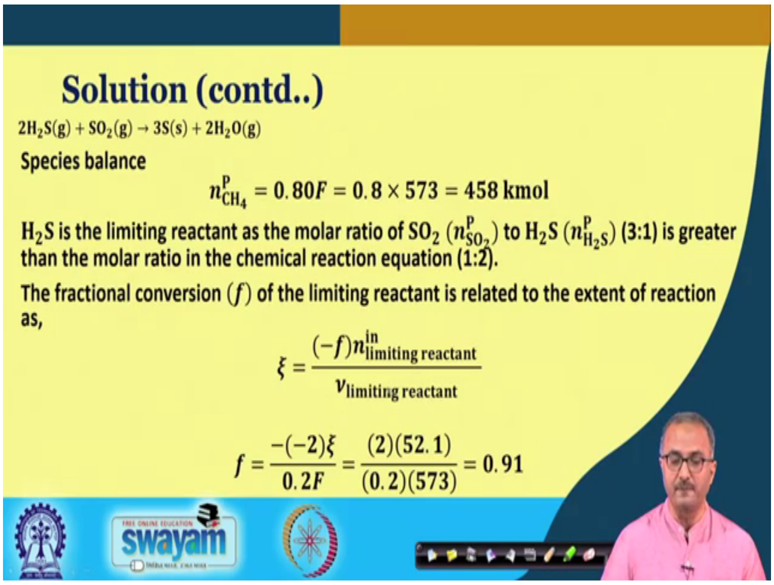

Now, we go to the next problem. Now, here we have been asked to find out the fractional conversion. And this fractional conversion can be correlated with the extent of reaction like this. And I am putting all these equations without any kind of derivation, because these are not required in this particular course. And these are taught separately in other course on reaction engineering, so that those things are not needed for you. It will sufficient for you if you just know the final relationships between the extent of the reaction and that fractional conversion. So, here this is the particular formula for this and you just find the value of F by plugging in the values of the various things. And in for limiting reactant, you just see that you have it for the H 2 S. So, you plug in the values over here, and you will get the fractional conversion of the limiting reactant as asked in the question.

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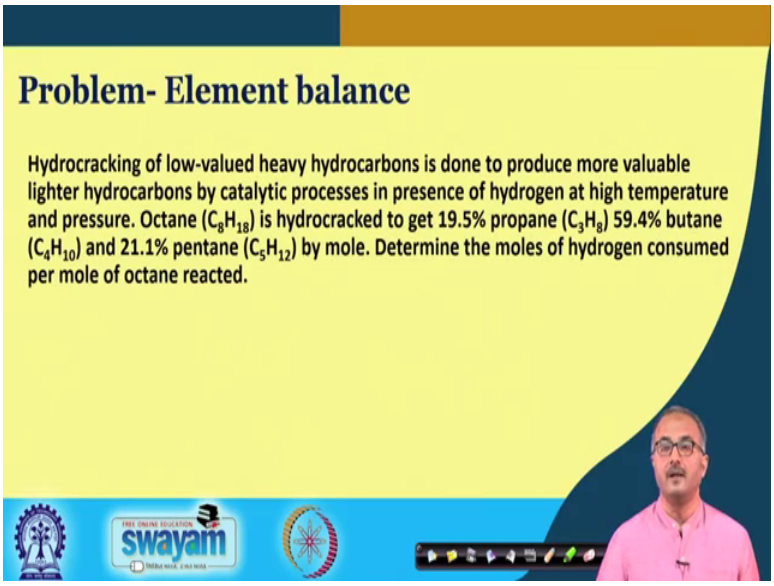

Our next problems relates to element balance. So, first let us look at the problem, and then we shall see what we mean by element balance, and where do we need this elemental balance because so far we have not done any elemental balance we have been doing some species balance or overall mass balances ok. So, let us see that we have a problem of hydrocracking. Hydrocracking is a very important refinery process which is used to convert the low-valued heavy hydrocarbons to more valued lighter hydrocarbons by some catalytic process in the presence of hydrogen that gives the name hydro ok. Cracking means breaking up a bigger molecule into smaller molecule that is cracking. So, we have a hydrocracking, the cracking in presence of hydrogen, and this requires a high temperature pressure ok. And this is done catalytically.

Now, it is said that octane that is C 8 H 18 is hydrocracked to get a lower hydrocarbon that is 19.5 percent of propane that is C 3 H 8, then 59.4 percent butane that is C 4 H 10 and 21.1 percent of pentane that is C 5 H 12 by mole. Now, please understand that if even if you are not told that percentage by mole or mass by default whenever it is a gas we take the percentage composition as in terms of the moles. Whether, whereas, in case of the liquids and solids when nothing is given we take the percentage as mass ok, this is the general convention. So, we have been asked to determine the moles of hydrogen consumed per mole of octane reacted ok.

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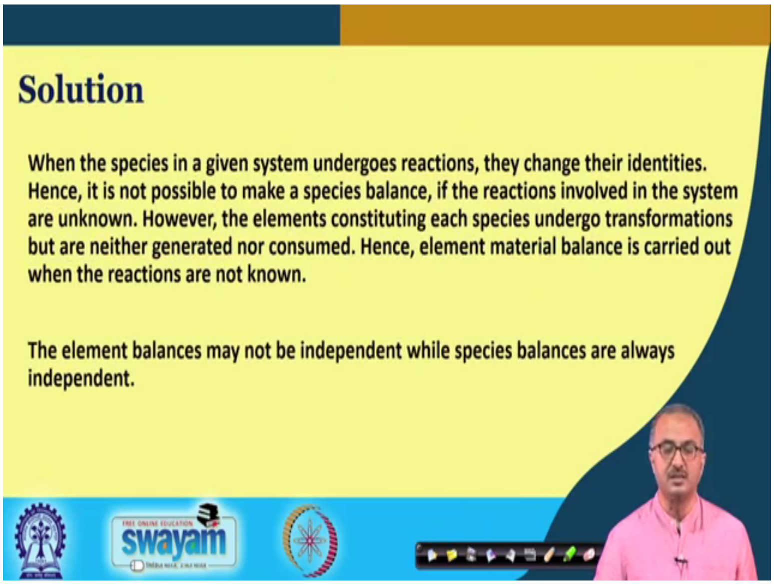

So, first let us see the element balance. Now, what we have done so far, we have done the species balance. And we can always do the species balance. And just species balance when we are doing and if we have some consumption term or generation term, and if we know the particular reaction then we can handle the species balance. But many a times it is found that the exact reactions are not known. What we only know, we know only the feed analysis and the product analysis. So, in that case how do we apply the material balance?

So, what is done in this instead of writing the species balance, what we do, we write the element balance, because we know that this elements will not be created or destroyed. So, what happens that whatever elements even if the species undergoes some kind of reaction and then it loses its identity, but the elements involved will not go anywhere, they will just simply go from one type of molecule to another type of molecule.

So, in that way we find that the elements will remain conserved. So, in those cases where we do not have the reactions, then there we use the element material balance ok. One thing is this element balances may not be independent, whereas the species balance may will always be independent, because the elements independent means you will find that in several reactions the same kind of element will be present. So, they are not independent ok.

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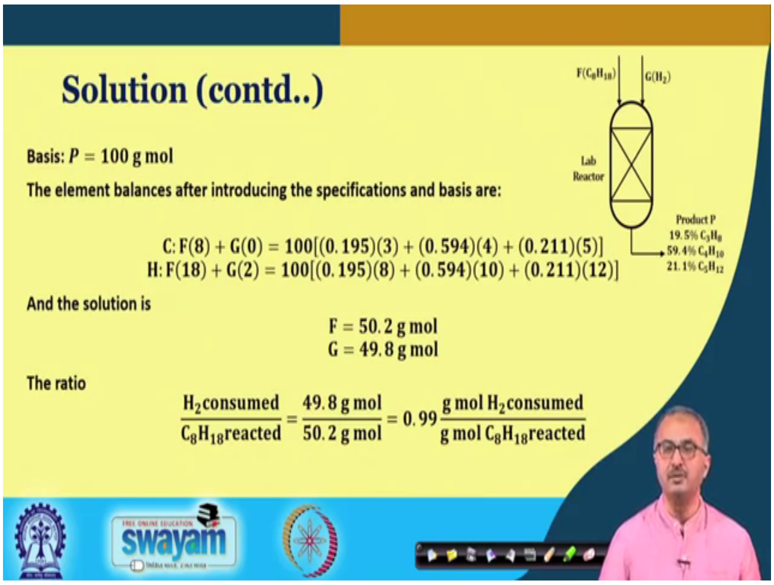

Now, let us come to our problem. First let us look at the particular system we have. Here we have the hydrocracker. And here we have the feed one feed is going that is the C 8 H 18 that is the octane. And along with that we have the hydrogen that is represented by G. And we have the product here, and the product we have the propane, butane and the pentane ok.

Now, what we do we take the basis as one of the product as 100 gram mole ok. And now whatever calculations we shall do, we shall do on the basis of this 100 gram mole. So, first let us do the elemental balance. So, for the C balance, now C balance what you find right in this in the feed we have 8 molecule 8 atoms of C elements of C. So, we are writing F as 8. And in the G that is in this particular stream we do not have any C, so we are putting this as 0. The and this is the this is the total amount of C carbon that is going into the system.

And what is the amount coming out of the system? So, we have to see that how much carbon is associated with each of the product streams. So, what we find with the propane we have 3 numbers of carbon, with the butane we have 4 number of carbon, and with pentane we have 5 number of carbon ok. And these are the respective compositions and we have the taken that 100 gram mole.

Now, please see that for the gases, when we assume that the gases are ideal, the mole fraction is same as the volume fraction ok. Now, here we are taking the moles. So, in this

100 gram mole, we have all these percentages of this particular product ok. And we are just this is the we are just multiplying with the number of gram moles to get the total number of gram mole. And now we have two equations and two unknowns, and we can solve these two ideally. And we one we do that we find that we are getting this much of feed, and this that this much of octane and this much of hydrogen for 100 gram mole of the product ok. That means if you take it to be any other 1 gram mole, you simply have to divide it by 100 ok.

Now, once you get this, it is the very easy to find out that how much hydrogen is consumed for amount of this. So, you can see easily from this particular thing that how much hydrogen has gone into these products, so that is the amount of hydrogen that has been produced. And this see that this is the 49.8 gram mole that is the that has been consumed, and this is the amount of this octane that has gone into. So, for per unit gram mole of octane, this many gram moles of hydrogen have been consumed. So, you can see that this is the very straightforward way of doing this kind of a problem.

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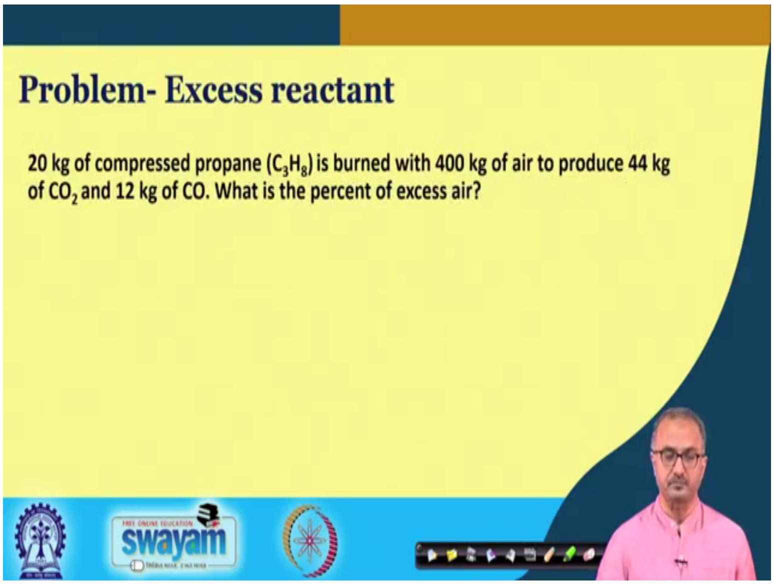

Next we come to another problem which involves excess reactant, because many a times when we carry out some reaction, we put excess reactant because it may be so that if you put the exact amount it may be so that all these things may not get reacted properly, therefore various reasons in the particular system. So, we put something in excess. So, here we have a problem in which that for 20 kg of compressed propane is burned with

400 kg of air to produce 44 kg of CO 2 and 12 of kg of CO. So, what is the percent of excess here? Now, what is air doing here? Air is basically a source of oxygen ok. So, and you know that air contains in majority nitrogen about 78.8 to 9 percent, and oxygen is next about 28.8 or 9 percent ok. So, these are the major products.

And roughly we can take that many a times we take the air to be a binary mixture of oxygen, nitrogen, taking nitrogen as 79 percent by volume and oxygen a 21 percent by volume. And we do not get pure oxygen for combustion always, because pure oxygen is very costly also because we have to separate oxygen from the air. So, it becomes very costly of air. So, many a times for combustion purposes of oxygen purposes we use the air.

But in that what happens that, the because it diluted because of the large amount of nitrogen present ok, but many anyway we do this kind of thing and whatever stoichiometric amount of oxygen is needed that will be supplied through this air. And now when you are using this air, we also have the problem of handling more volume than what exactly is required for the particular combustion process.

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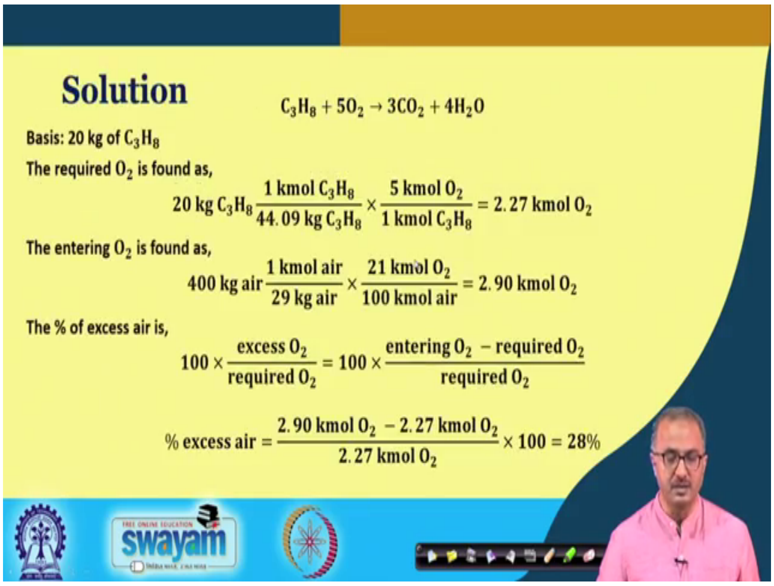

Now, first we look at the particular reaction. Here, we have that we assume that the reaction is completely done. So, any kind of hydrocarbon when is getting reacted with oxygen, it will produce all the carbon dioxide and H 2 O. So, here because we have been given that 20 kg of propane is there. So, we put this as the basis. And now we find from the stoichiometry how much is the amount of oxygen required.

So, what we find 1 mole of propane needs 5 moles of oxygen for its complete conversion. So, that is what we do that we have 1 kilo mole of this propane and that needs 5 moles of oxygen, and we what we do that we convert them into there by dividing with their molecular weight, we convert in to mass, because our basis is in mass ok. So, now we simply multiply the mass of the propane to obtain the amount of the oxygen.

And similarly this is the amount of oxygen that is entering the system. We have been given that 400 kg of air. And in 400 kg we know that 21 mole percent is there; that means, 21 kilo mole per kilo 100 kilo of air, and we divide it with the molecular weight of air to and then we get the in terms of the per kg of the air, and multiply with the amount of air that is provided. So, we get this many moles of oxygen that is entering along with the 400 kg of air.

Now, this is the amount which is needed stoichiometrically and that and this is the amount we are sending in the system. So, this 2.9 minus 2.27, this is the excess amount of the oxygen we are giving to the system. So, percent of the excess air is that 2.9 minus 2.7 divided by the stoichiometric amount that is 2.27 into 100. So, we are finding that, we are sending 28 percent excess air ok. And here you can see that how we are calculating this excess air amount per mole of oxygen required ok.

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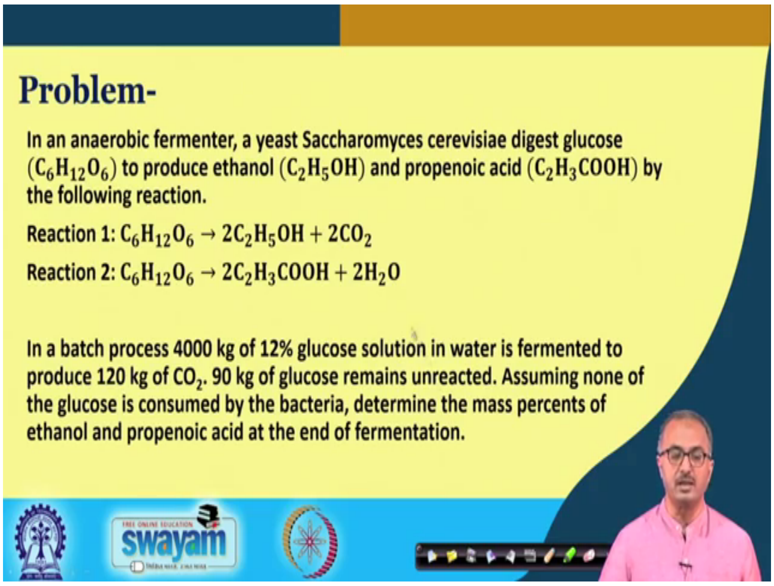

Next we come to another problem. In this we have an anaerobic fermenter. And we are using some kind of yeast this is Saccharomyces cerevisiae and this is the baker's yeast to digest glucose to produce ethanol and propenoic acid. So, these are the two reactions which are going on. So, from the first reaction, we are getting the ethanol; and from the second reaction we are getting the propenoic acid. So, it has been mentioned that for 4000 kg of 12 percent glucose solution in water that means, we are given the composition of the feed that is a 12 percent glucose and that means, rest of that means, 100 minus 12 that is a 88 percent is the amount of the water is fermented to produce 120 kg of carbon dioxide.

Now, 90 kg of glucose remains unreacted. So, assuming none of the glucose is consumed by the bacteria that means, the bacteria are not eating up any of the glucose. So, everything glucose only goes to produce these two compounds. Determine the mass percents of ethanol and propenoic acid at the end of the fermentation.

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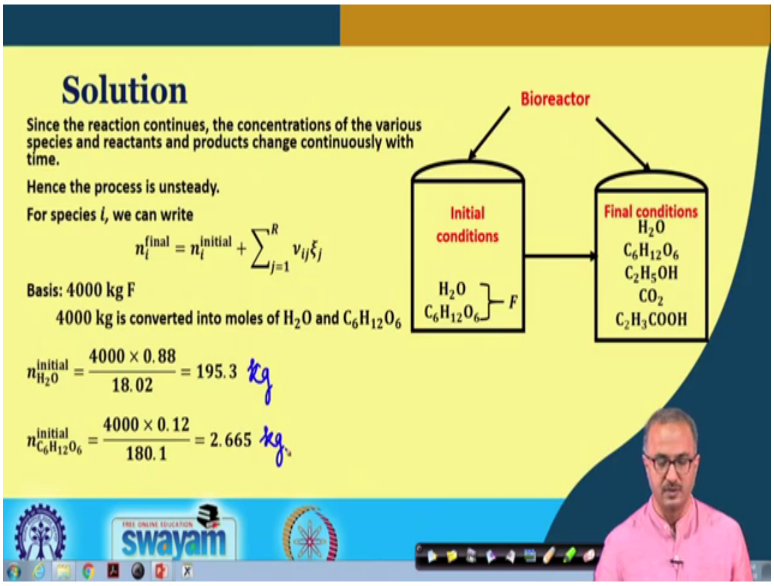

So, here we have that since the reaction continues we put this thing that is the bioreactor. So, this is the initial condition with the feed, and this is the final condition whatever have been the product. So, because the reaction is continues, so it is not that we are as long as the things are these reactants are not exhausted, the reactions will go on ok. So, we have basically an unsteady state process. And due to which how to find this the product composition will keep on changing. So, at a given time instance, what we do, we can find out the final amount that what is the initial amount plus whatever is the extent of the reaction.

Now, here you see that for the product side because nu will be that is the stoichiometric coefficient from a given reaction j will be positive. So, it will lead to increase in the n i final. Whereas for the feed side this nu is negative so we will automatically get a reduced amount of the reactants at any given time after the start of the reaction.

So, now we take the basis as 4000 kg of feed as given in the problem. And this 4000 kg is converted in to moles of H 2 n C 6, this glucose. So, from the percentage we know that 88 percentage. As I told you that for liquids by default we take it to be the mass percentage. So, we get the total amount that is 195.3 kgs of the H 2 O, and this 2.665 kgs of the this glucose. So, this is kg of water and this is kg of glucose ok.

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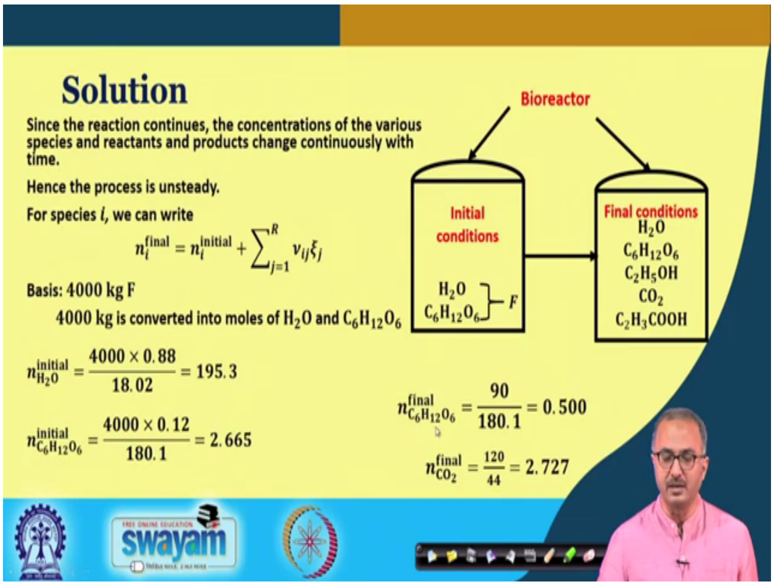

After this what we do that we simply find out the number of moles. And for this what we do we just simply divide the amount of the final amount of the glucose that is 90 kg as mentioned in the problem with the molecular weight of this 180.1 and similarly we do it for the carbon dioxide. So, we get the final amount of these two components.

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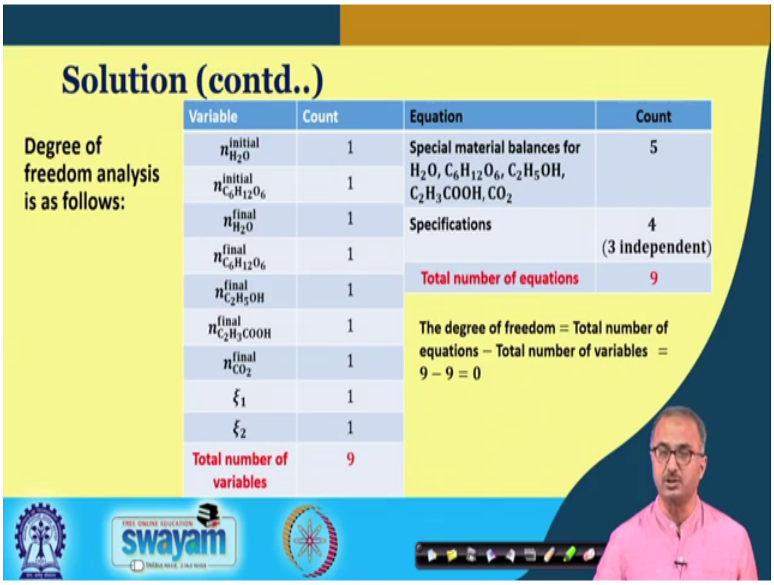

And then we do the degrees of freedom analysis. I you can see that we list out all the variables over in this particular table. And we make the count of them, and we found the total number of variables is coming to 9. And then we do the counting of the equations, so we write all the material balance for each of the species and all the specification variables. Here we have the 4, now three independent means that in this specification variables either you can mention the amounts of the glucose and water going into the system.

And in that case, you do not need to mention the total amount of the feed or you can do what you can mention the total amount of feed and the percent composition of any one of the things either glucose or the H 2 O. We need not mention all the three ok. Then it will not be independent and for these equations we know these have to be independent specifications, so that is why to tend three independent. Now, we see the total count of the equations come to 9, and total number of variables also come to 9. So, the degrees of freedom is coming to 0 that means we have the this particular problem is well posed ok.

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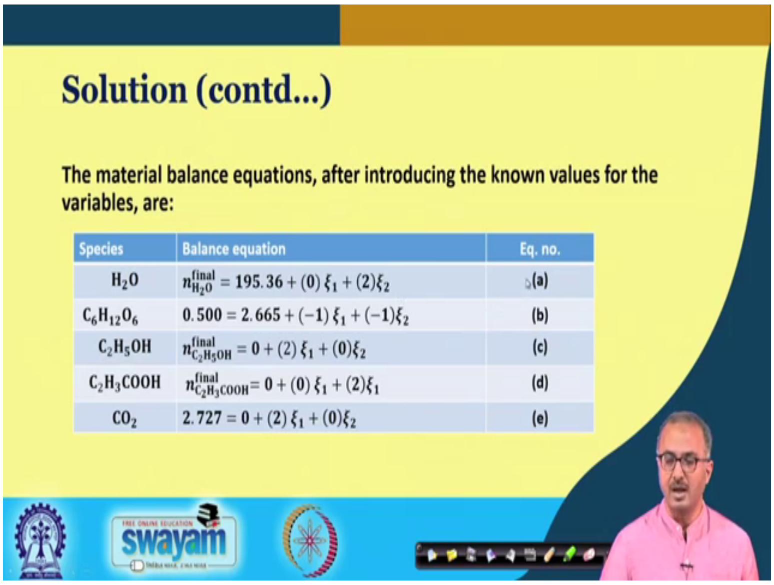

And we have unique solution. Now, what we do we write all the species balance equations for each of the species in terms of the extent of the reaction. And these you can write very easily from the definition of the extent of reaction. And we have to please just one thing is this here you have to just take care that any species like for glucose will be involved in both the reactions ok.

On the other hand ethanol and the propenoic acid will be there will only one of the reactions ok. So, accordingly we will find for some reactions like some reactions it is coming only one reaction, some of them we are coming both reactions. So, that is why and these are independent reactions. So, we are having independent zeta 1 and zeta 2, and here we are naming the equations.

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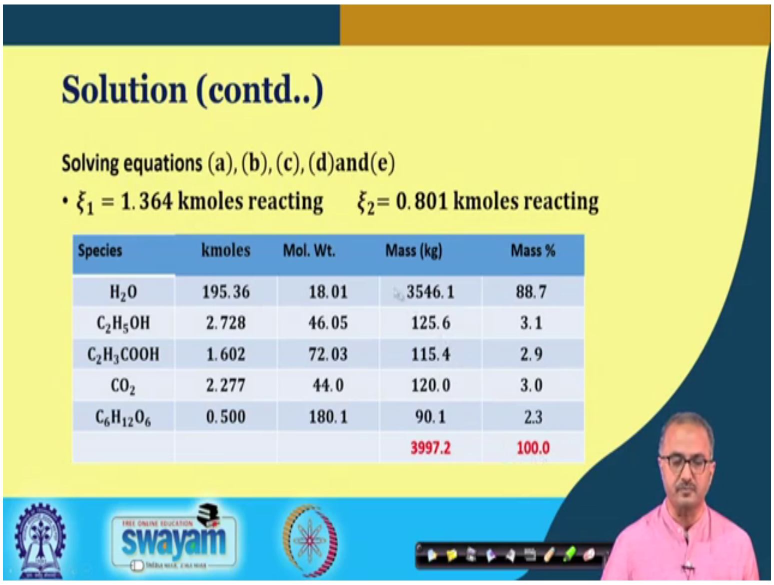

Species	kmoles	Mol. Wt.	Mass (kg)	Mass %
H_2O	195.36	18.01	3546.1	88.7
C_2H_5OH	2.728	46.05	125.6	3.1
C_2H_3COOH	1.602	72.03	115.4	2.9
CO_2	2.277	44.0	120.0	3.0
$C_6H_{12}O_6$	0.500	180.1	90.1	2.3
			3997.2	100.0

And now we have to solve this equations the solution is pretty simple. So, I am not going into detail of the solution. So, these are simply algebraic equation. And you can solve them one by one. You can find out the zeta 1 and zeta 2 easily. Zeta 1 and zeta 2 can be found out from this equation and this equation that is the species balance for glucose and carbon dioxide, you can find zeta 1 and zeta 2. Once find zeta 1 zeta 2, then you can put their values in the other three equations to get the amounts of the other components.

So, here we have just put all those things here. So, we have convert first we have kilo mole, then we have the molecular weight to make them the mass. And from that mass it is the total mass. And from this mass we divide each of the masses with this total mass to get the mass percentage. And after getting the mass percentage to check that whether the solutions are right or not, we add it up, and we find yeah they are adding up to 100, that means, which shows that the calculated mass percentages are right.

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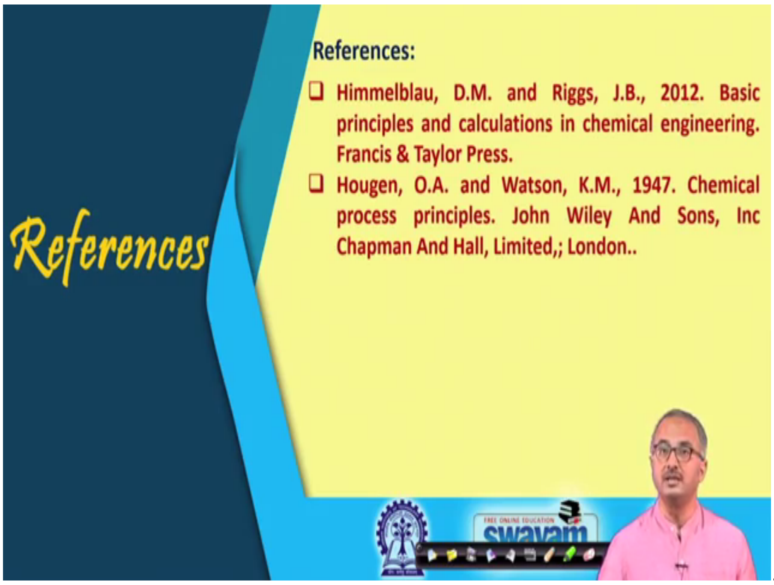

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More of these kind of problems and kind of theories will be found in these two books.

Thank you.