Material and Energy Balance Computations
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Lecture –23
Multiple Reactions and Reactive Process Balance

Hello everyone, welcome back once again in the NPTEL online certification course on Material and Energy Balance Computations. We are in module 5, where we are learning the balances on the reactive system. Now in the last class we have seen multiple reactions and how we can apply the balances on such multiple reactions. We have seen 2 approaches out of the 3 that are molecular species balance and atomic species balance.

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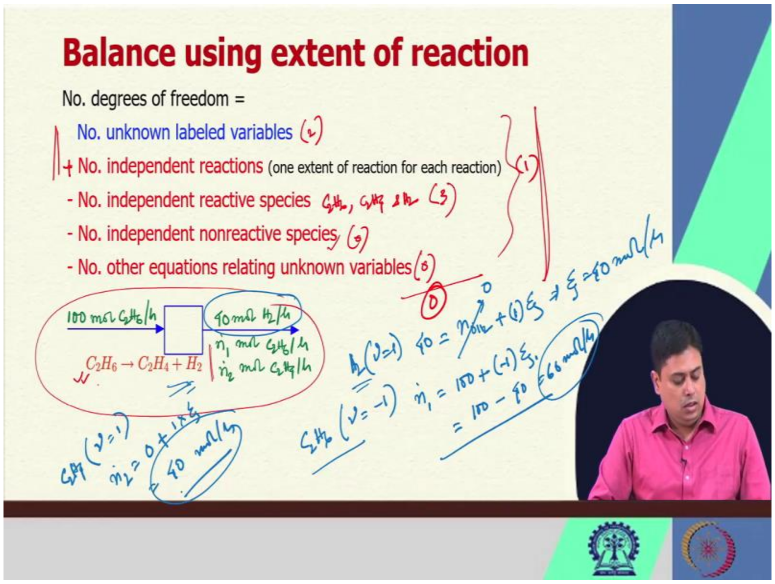

And today we will see the balance using extent of reaction for the same example that we did in the last class. Now while doing the extent of reaction, by now we have understood the concept of extent of reaction. So, any problem when we try to solve using the concept of extents of reaction even in multiple reactions the first thing that we do is the degree of freedom analysis. Now in this case likewise the previous 2 examples I gave that is on molecular species balance and atomic species balance.

Here the degrees of freedom are calculated based on these parameters which are that the first thing we identify the number of unknown labelled variables then from there we subtract the number of independent reactions. We have already seen the concept of independent reactions. Now these independent reactions actually result in individual extent of reaction. So, we define extent of reaction for each individual reaction that is why it is then subtracted from the number of unknowns that we have.

And then we subtract further the number of independent reactive species that we have in the system, the number of independent non-reactive species that are there in the system and if there are any unknown variable that are related with some additional information that is the number of other equations relating unknown variables, by doing so, we then find out what is the number of degrees of freedom.

So, let us apply this understanding to the problem that we solved in the last class as well using molecular species balance and atomic species balance. Now here the same schematic our objective is to find out $\dot{n}_1$ and $\dot{n}_2$, for that we are doing the degrees of freedom analysis now using extent of reaction. So, here what should we do at first, what we can understand that the number of unknown labelled variable here we have 2, then the number of independent reaction we have only one.

So, here we have only one independent reaction in the system the number of independent reactive species that we have here, we have 3 reactive species that are C_2H_6, C_2H_4 and H_2. It is recommended that we write just beside these phrases and we clearly identify what are the known and what are the unknown in such cases. Next we have number of independent non-reactive species. Now in this system there is none.

So, here we had 3 reactive species. So, the thing that we have it is. So, here it is basically a typo it would be the number of independent reactions that we have that would be in addition like we have seen for the non-reactive reactive species balance using molecular spaces. So, in molecular species balance we have seen that the reaction adds a level of complicacy in the problem and that is by the number of independent reactions that are happening.

So, similar to that concept here we have number of unknown labelled variables + the number of independent reactions that are happening. So, what we have here that means 2 + 1 – 3 because there is no other thing or no other information that has been given. So, that means what do we have here for the same problem we can see that using extent of reaction we have degree of freedom as 0. So, once again let me repeat the process.

It is the number of degrees of freedom is actually the number of unknown labelled variable + the number of independent reactions in the system – the number of independent reactive species – number of independent non-reactive species – number of other equations relating the unknown variables this gives the summation of all these including the sign gives us the degree of freedom using extent of reaction.

So that means in this case we have zero degrees of freedom even using extent of reaction. So, that means we can solve the same problem using extent of reaction. So, in this case what will happen if we now try to apply extent of reactions, how it would look like. Now in this case if we look at hydrogen. So, here the stoichiometric coefficient is positive one because it is a product.

So, that means here since it is known parameter at the outlet we are taking that at first. So, the outlet H_2 we have 40 mol/h that = the initial or the input feed that we have. Now here this is H_2 but here it is none because there is no hydrogen in the feed + we have stoichiometric coefficient that is one in this case from the stoichiometry and since it is a product it is positive one and the extent of reaction or say since here we have only one reaction we can just mention that as ξ.

So, which means we have ξ = 40 mol/h. So similarly now if we apply this for C_2H_6. In this case it is – 1. So, which means the thing that we have at the outlet which is $\dot{n}_1$ = the amount of feed that goes in with respect to C_2H_6 which is here 100 + (– 1) and then we have ξ. So, which means we have 100 – 40, which is 60 mol/h.

Similarly if we apply for C_2H_4 this is positive one because this is a product in this case $\dot{n}_2$ = 0 because there is no input + 1 × ξ = 40 mol/h. So, which means we have this identical result that is n_1 60 mol/h and n_2 40 mol/h even using extent of reaction. So, that means using 3 different approaches for a single problem results the same or the identical answers and it should be.

But now we have understood that molecular species balance is relatively complex than the other 2 method that is the atomic species balance and extent of reaction.

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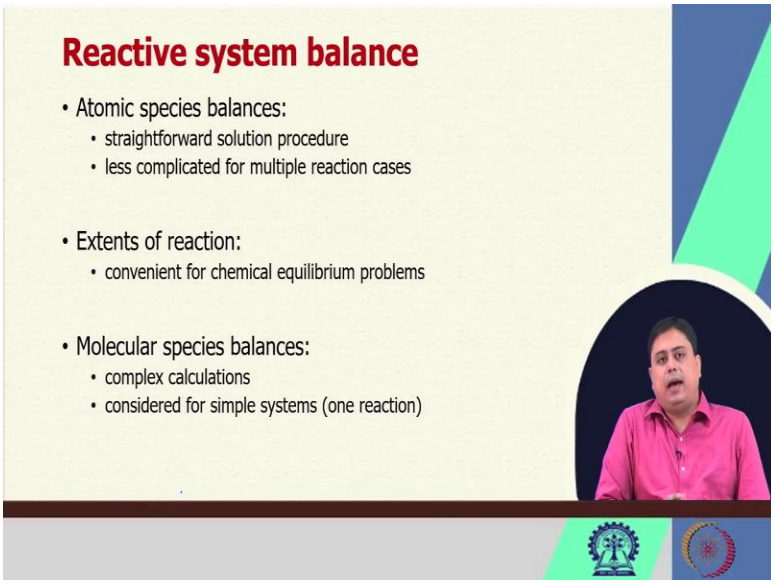

So the reactive system balance we have seen these 3 approaches that is atomic species balance, extent of reaction and molecular species balance. Atomic species balance is straight forward and simple to implement because it is only input = output that we have to look for, for the atomic species and it is less complicated, when I mean less complicated we realize this when we apply this for multiple reactions.

For single reaction or for one reaction even the molecular species balance is kind of a similar in the terms of complicacy. So, the extent of reactions these are the recommendations that it is convenient for chemical equilibrium problems. So, whenever we find any chemical equilibrium problems in our system we typically apply extent of reaction method to solve for the material balances in reactive system.

Molecular species balance is relatively complex than the other 2 and typically we apply this when we have simple systems which is kind of one reaction in the system. So, the point is that whenever the problem statement would be given to you which would or which may involve multiple reactions because most of the processes that we have commercially involves side reactions.

So, if you encounter multiple reactions and it has not been specifically asked that solved by this method or that method typically go for the atomic species balances when there are multiple reactions.

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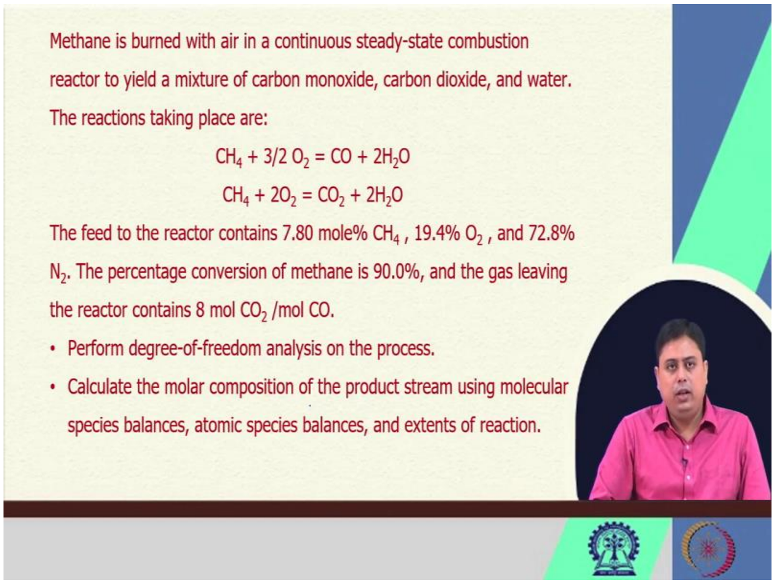

So, for example if we look at this problem statement where now we have 2 reactions happening parallel that is methane is burned with air in a continuous steady state combustion reactor to yield a mixture of carbon monoxide, carbon dioxide and water. The reactions that are taking place are given in this set. The feed to the reactor contains 7.8 mole% methane 19.4% oxygen and the rest nitrogen.

The percentage conversion of methane is 90% and the gas leaving the reactor contains 8 mole carbon dioxide per mole of carbon monoxide. We have to perform the degree of analysis of the process and we have to calculate the molar composition of the product stream using 3 methods that we have learnt. So, by doing so, we will see that why I am always mentioning that molecular species balance is relatively complex to implement or its relatively difficult not very difficult but its relatively than the other 2 methods.

So, the first thing that we do is we draw the flowchart. So, once again quickly have a look at the problem statement that we have 2 reactions. The feed composition is known, percentage conversion of methane one information is given, and the other information given is the gas leaving the reactor contains a certain mole ratio of carbon dioxide to carbon monoxide. We have to calculate the molar composition of the product stream.

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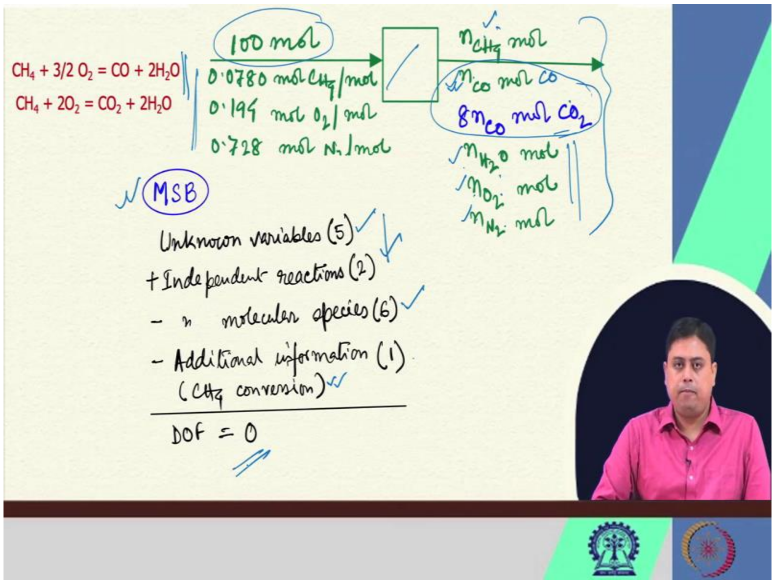

So, our basis of calculation the logical one is 100 mole because all the composition is given in mole percentage. The reaction is happening in the reactor and we have the unknown feed compositions out of which, one information we have directly translated on the flow chart which is the mole ratio of CO and CO_2 it is said that 8 moles of CO_2 is formed per mole of carbon monoxide. So, if nCO is the moles of carbon monoxide 8 times of that is the number is the amount of mole of carbon dioxide and rest are unknown.

So, which means for this process we can identify we have 1, 2, 3, 4, 5 unknowns. Now the first step is we do the degree of freedom analysis. The molecular species balance or abbreviated here as MSB. So, here what we have the unknown variables 5 that we have counted 1, 2, 3, 4 and 5 + the number of independent reactions that are happening in the system, we have 2. Independent molecular species in the system here we can see that we have 6 species that are clearly methane, carbon monoxide, carbon dioxide, water, oxygen and nitrogen.

So, we have 6 independent molecular species and we have another additional information that is the methane conversion that the percentage conversion to methane that is given in the problem statement which is said that the percentage conversion of methane is 90%. So, that is the additional information. So, which means 5 + 2 – 6 – 1 which is zero the degree of freedom by molecular species balance that means we can solve the problem using molecular species balance and the problem is solvable.

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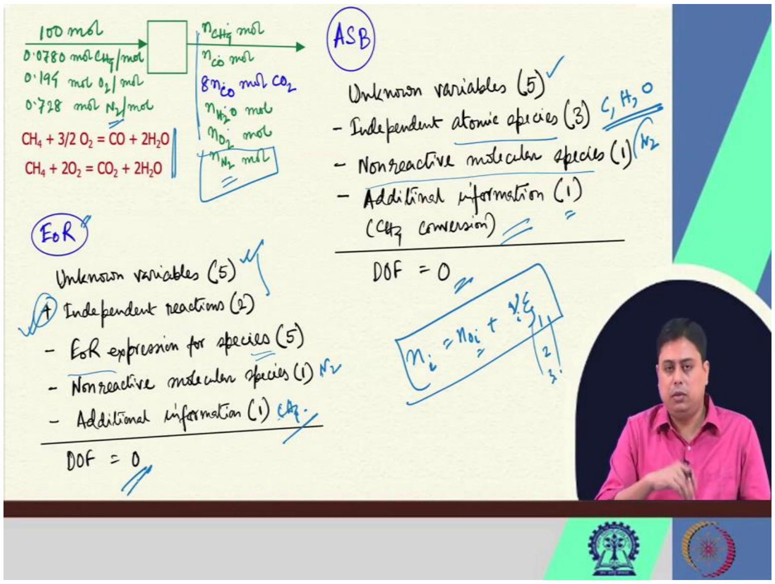

Similarly, now we look at the atomic species balance. In atomic species balance the unknown labelled variables remain same but here we find out what is the independent atomic species the number of independent atomic species. Now that is 3 here because it is C, H and O. These are the independent atomic species that we have in the system. The non-reactive molecular species the number we have is nitrogen because it is not taking part in the reaction there is no nitrogen in the stoichiometric reactions.

So, that is why it is considered as non-reactive molecular species not in the atomic sense. The species that are involved in the reactions in atomic species balance those are considered for atom as atomic species and independent atomic spaces. The rests that are not taking part we go ahead with the molecular species consideration for those cases and in addition to that we have the methane conversion information that is – 1.

So, this non-reactive species is basically nitrogen. So, that means our degree of freedom in this case is zero by atomic species balance. At the same time now we look at the extent of reactions abbreviated here as EOR the extent of reactions. Then unknown variables remains same we have 2 independent reactions. So, that is why it is added to the system the corrections that I made on the first slide that was a typo.

So, here we have + 2, 5 + 2 and then here we have the species that are involved in the reactions for which we can write the extent of reaction expressions that is the expressions that we had is 1, 2, 3 depending on the number of reactions for the ith species. Such kind of expressions how many we can write for this problem, we see that nitrogen is inert here. So, which means we have 1, 2, 3, 4, 5.

This initial 5 species for which we can write the extent of reaction expression and we have non-reactive molecular species one which is nitrogen and the additional information of methane conversion. So, 5 + 2 – 5 – 1 – 1 which is zero, so, a particular problem we have applied 3 different methods molecular species balance, atomic species balance and extent of reactions in all the 3 cases we see the degree of freedom is zero which means the problem is definitely solvable and also it is possible by all the 3 methods. Now we move on to the solution of the problem.

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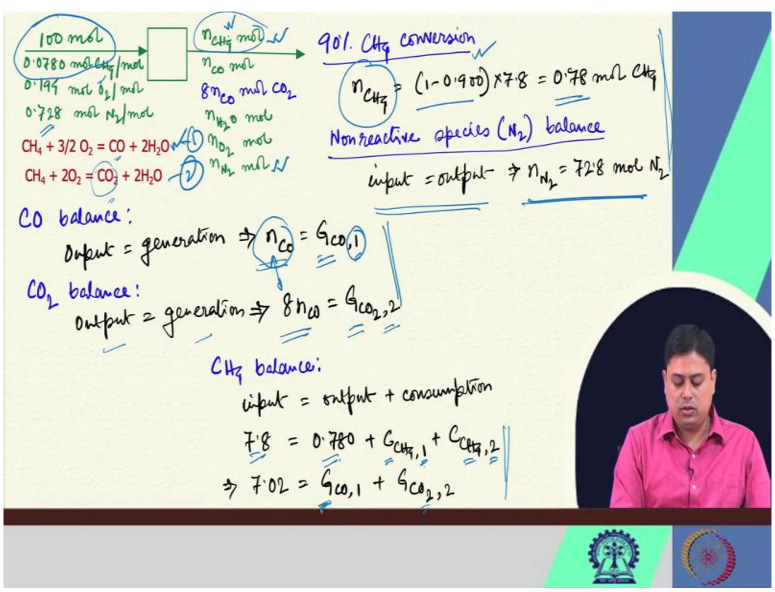

The first thing that we can do is the information that is given and the non-reactive species balance because it is common for all the 3 cases if we look at it. So, here there is non-reactive molecular species in this case there is non-reactive molecular species as well as here we have this independent reactions and the independent molecular species that we have. So, that means in the independent molecular species here is nitrogen is also included.

So, that means it is common in all the 3 cases. So, with the first additional information that we have that 90% methane conversion which means 10% is unconverted, if the 10% is unconverted that means it would leave the reactor. So, 10% of the feed which is one – the conversion fraction × the amount of feed that is there in the system that unconverted part will leave the reactor without any reaction.

So, which means the amount of methane that is leaving the reactor is 0.78 mole. So, that means we now know this value and again if we look at this non-reactive species balance which is common for all the cases as I mentioned and that is the input = output because it is a non-reactive species not taking part in the reactions. So, simple input = output the amount that comes in is 0.728 × 100 mole because 100 mole is the basis of calculation based on that basis of calculation the amount of nitrogen that would leave the system is 72.8 mole.

So, that means we now know 2 unknowns out of the 5 that we have. So, 1, 2, 3, 4, 5 unknowns we had and now we know 2 out of them. Now if we look at the molecular species balance because till this part it is common for all the 3 processes. Now say at first we apply molecular species balance. Now here if we start with the CO balance because the CO and CO_2 this molar ratio is given at the outlet.

So, that means if the CO balance and CO_2 these 2 will have the relation which is known to us. Now for CO in molecular species balance what is happening the output is the generation and this generation is happening from the first reaction only. So let us write that that the output = generation and the output amount is nCO mole which is G stands for the generation that we introduced in the last class that it is generation and consumptions like this we will distinguish.

So, here the generation of CO from the first reaction that means if we designate that this is the first reaction and this is the second reaction. Similarly for carbon dioxide it is output = generation that means output is 8 times of the amount that is going out in terms of carbon monoxide. So, we have 8 nCO = generation of carbon dioxide that is happening only in the second reaction because carbon dioxide is formed from the second reaction.

The reason of doing so, because once we know these amounts by stoichiometry we can find out the other component that is the amount of methane will be consumed to form a known amount of carbon monoxide and a known amount of carbon dioxide or say the amount of oxygen will become consumed to produce those amounts of carbon dioxide and carbon monoxide. So, which means now here if we now look at the methane balance.

So, methane here is the reactant, this reactant is the input = output + consumption in the reaction. So, here the input amount is 0.078 × 100 which is 7.8 + the output that we have which is number of moles that we already calculated here that is 0.78 + its consumption in first reaction C stands for the consumption of methane first reaction and consumption of methane in second reaction.

Now this is where this consumption is now related with the generation of carbon monoxide in the first reaction. So, we can see that to generate one mole of CO we require one mole of methane in the first reaction. To generate one mole of CO_2 we require one mole of methane in the second reaction this is where it is written. So, which means now if we replace these values that G CO,1 is nCO and G CO_2,2 is 8 nCO these relations.

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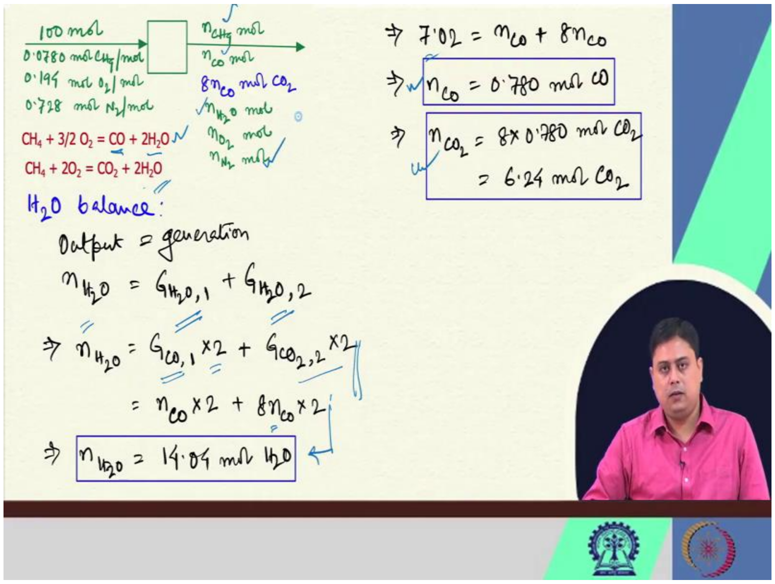

What we have that nine times of nCO is basically 7.02 that means we can calculate the amount of carbon monoxide and carbon dioxide subsequently because it is the 8 times of that value. Once we calculate that we then apply say the H_2O balance. Now H_2O balance we have only in the output. So, it must be equal to its generation. Now the amount it is being generated is from the first reaction and from the second reaction that would go out in the output.

Now similar to our previous discussion that we just did this for generation of one mole of CO in the first reaction it also generates 2 moles of water. So, that means the generation amount of CO would be × 2 for the first reaction and that would give us the amount of water being generated. Similarly in this case the generation amount of carbon dioxide × 2 times of that from the stoichiometry is the amount of water being generated.

We know the value of nCO we replace it here we find out the moles of H_2O. So, which means we now know n CH_4, nCO, nH_2O we also knew nN_2 the moles of nitrogen from the molecular species balance it is a non-reactive species.

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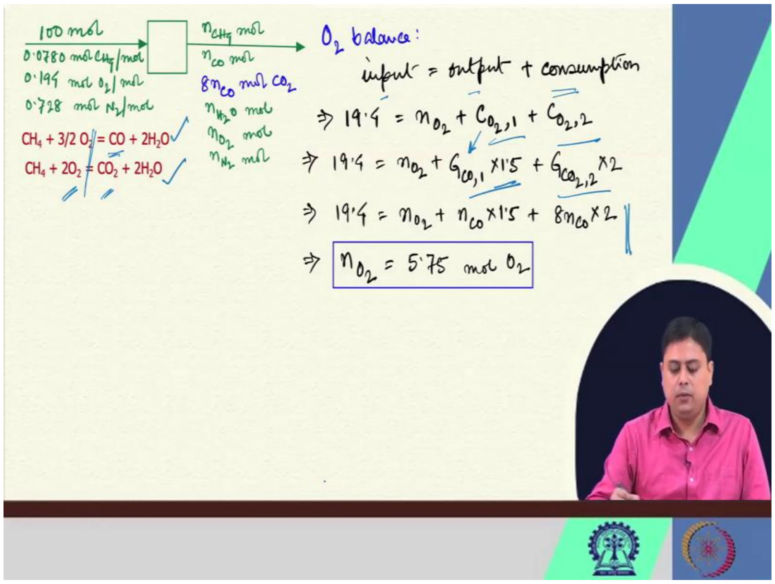

So, the remaining part is the oxygen balance we do it as discussed. So, it is input because here it is the reactant. So, we have input = output + its consumption. The consumption in the first reaction, consumption in the second reaction first and the second reactions. Now this is further related with the generation of carbon monoxide and carbon dioxide. In the first reaction for generation of one mole of carbon monoxide we require 1.5 times of oxygen which is the amount of consumption of oxygen in the first reaction.

In the second reaction we require 2 times of the amount of CO_2 being generated. So, which means what we are doing here we are converting all the unknowns in terms of nCO, nCO is known. So, we can have the value of nO_2.

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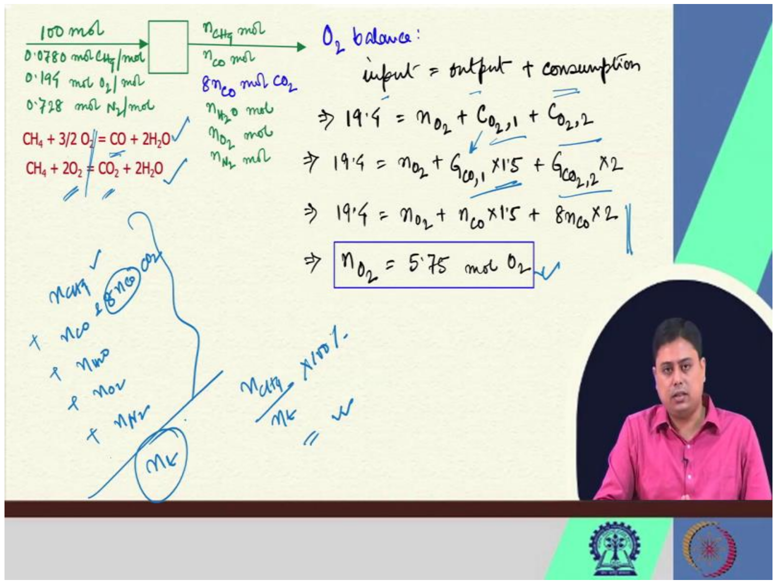

So, which means what we have is the values of nCH_4 that is known. Now nCO and so, as the 8 nCO which is the moles of CO_2. We now know the value of H_2O, O_2 as well as N_2, we do the summation of all these we get the n total. Once we have the n total we divide the individual species to get the percentage moles in the product stream. So, the mole percent of the product stream can easily be calculated.

Because we have now calculated all the individual species this algebra I leave it to you because it is pretty much straight forward and simple. So, I hope you have understood the application of molecular species balance in the case of multiple reactions and how stoichiometry helps. In the next class we will see the example of atomic species balance for the same problem as well as the application of extent of reaction. Till then, thank you for your attention.