Material and Energy Balance Computations
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Lecture –19
Introduction (Contd.,)

Hello everyone, welcome back once again in the NPTEL online certification course on Material and Energy Balance Computations. We were discussing the fundamentals of chemical reaction stoichiometry. We have learnt what is limiting reactant what is excess reactant what is stoichiometric coefficient, what is stoichiometric ratio. Now based on these concepts we try to solve one problem.

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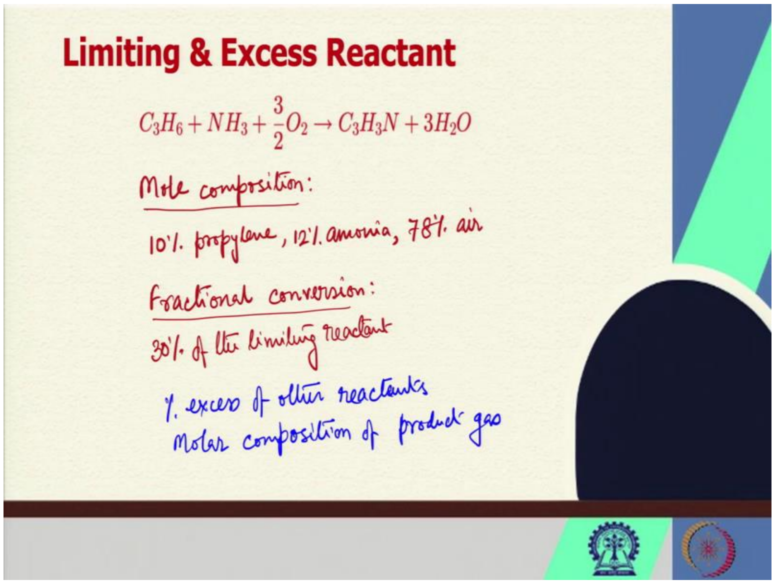

We initiated this and we will solve it now. So, the problem was like this that this reaction is happening in a reactor where the feed mole composition is this. The fractional conversion is mentioned as 30% of the limiting reactant, we had to find out at first the percent excess of other reactants which means at first we have to find out what is the limiting reactant.

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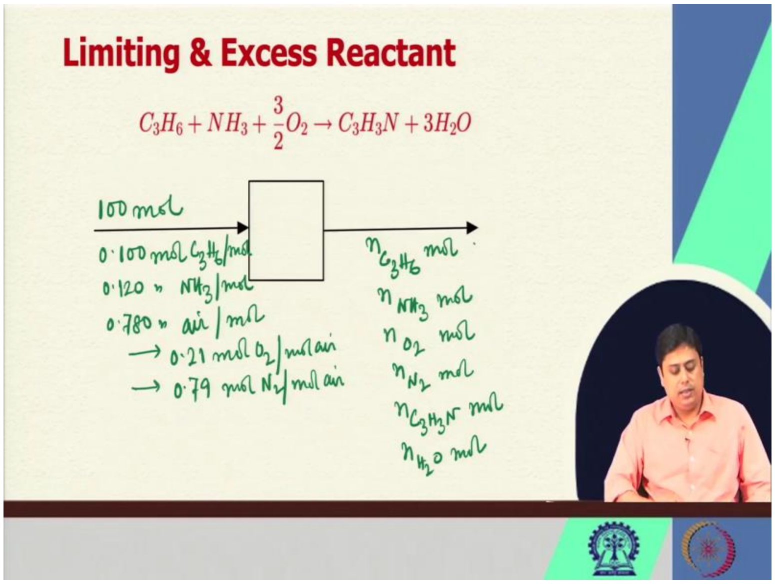

Now this is the scenario we discussed that this is the flowchart of this problem and why there will be so, many constituents of the species in the product stream.

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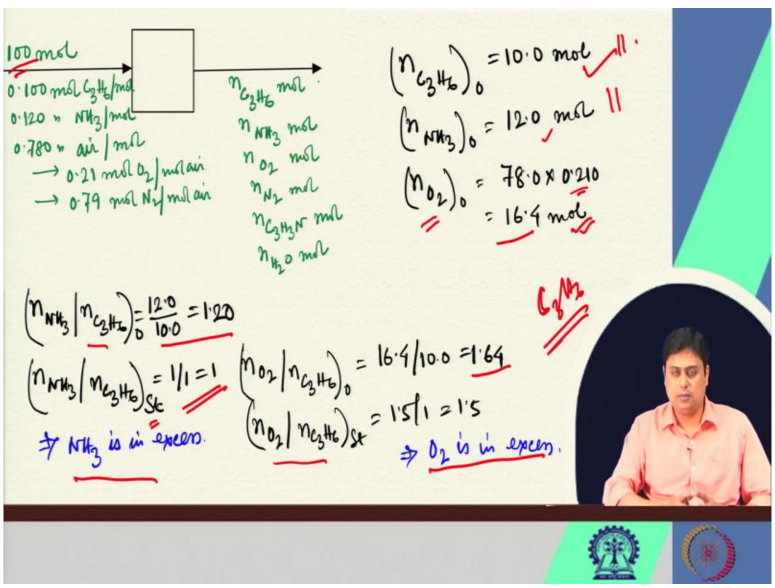

So, then what happens is that if we look at the initial feed composition based on the basis of calculation of 100 mol. So, the nomenclature that we can follow here is that $n(C_3H_6)_0$ subscript 0 means at the feed condition or at the inlet condition which are 10 mole when the total number of mole being fed is 100 because this is 10%, 12% and oxygen is the 21% of the air and the air itself was 78%.

So, this is the amount of oxygen that are now fed in the system. Now if we have to find out what is the limiting one we have to look into at first the stoichiometric ratio. The stoichiometric ratio is here the number of moles that is required for this reaction with respect to NH_3 here and C_3H_6. So, these are fed with a ratio of 1.2 :1 for NH_3 : C_3H_6. So, which means we have 10 moles in the feed 12 moles of ammonia in the feed, the ratio of these 2 that means the ratio of number of moles of ammonia fed with respect to number of moles of C_3H_6 is 1.2.

But stoichiometrically if we look at the reaction in a balanced form we see that one mole of NH_3 is required per one mole of C_3H_6. So, which means the stoichiometric requirement is 1 the stoichiometry ratio of NH_3 : C_3H_6 is 1. So, st here stands for the stoichiometric ratio but it is fed as 1.2 : 1. So, which means obviously NH_3 is in excess. So, we have 3 reactant in which we now see that NH_3 is in excess with respect to C_3H_6.

Similarly we look for oxygen with respect to C_3H_6 in the feed we can easily see that it is 16.4 : 10 which is 1.64 : 1 but stoichiometrically we need 1.5 mole of O_2 it is needed per mole of C_3H_6 here I am not writing consumed or generated which why should it is consumed per mole of C_3H_6 consumed. So, which means here the ratio stoichiometric requirement 1.5 : 1 but we are supplying 1.64 in this problem.

So, which means O_2 is in excess with respect to C_3H_6 which means C_3H_6 is our limiting reactant. So, C_3H_6 on this problem is fed as limiting reactant or for this problem we should consider C_3H_6 as the limiting reactant.

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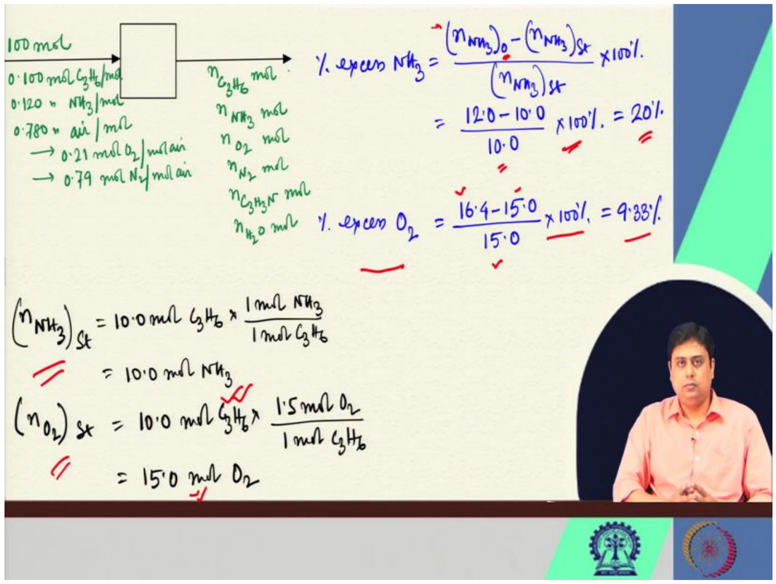

But then the others are in excess. So, this is what is the stoichiometric requirement 10 mol NH_3 it is apparent now because what happens here we are feeding the system with 10 mol of C_3H_6. So, it is the limiting reactant the other reactants should be in excess of the stoichiometric requirement with respect to this limiting reactant that means the stoichiometric requirement of NH_3 is 10 mol because the ratio was 1.

The stoichiometric requirement of oxygen like we have seen earlier it is the 1.5 times of the SO_2 moles which is 15 moles of O_2. So, these are the stoichiometric requirement and now we see that how much has been fed because there we calculate the percentage excess. So, again the zero that is for the inlet or the feed condition. So, the amount of feed with respect to NH_3 – the stoichiometry requirement is the excess and in order to find out the percentage excess we divide that with the stoichiometric number or the stoichiometric demand multiplied by 100.

So we see that we have 20% excess NH_3 is being fed to the system. Similarly what is the percentage excess of oxygen because once we have percentage excess of ammonia and we have realized the percent the limiting reactant as our C_3H_6 that means along with ammonia there will be percentage excess of oxygen. So, similar to our calculation previous calculation for ammonia we can write that percentage excess oxygen is its inlet amount or the feed amount – the stoichiometry requirement divided by the stoichiometric requirement multiplied by 100% which is around 9.3%.

So, I hope this part is clear to you that how we identify which one is the limiting reactant. Now this is quite elaborative this is shown with a quite elaboration based on the 3 reactant species there can be multiple or more than 3 species in a reaction. This is how we zero down on the limiting reactant. Sometimes it is quite apparent and intuitive from the reactions balance reaction again in order to find out which one is the limiting reactant you must balance the reaction or means you have to write the stoichiometric equation and then you should find out what is the limiting and which one are the excesses.

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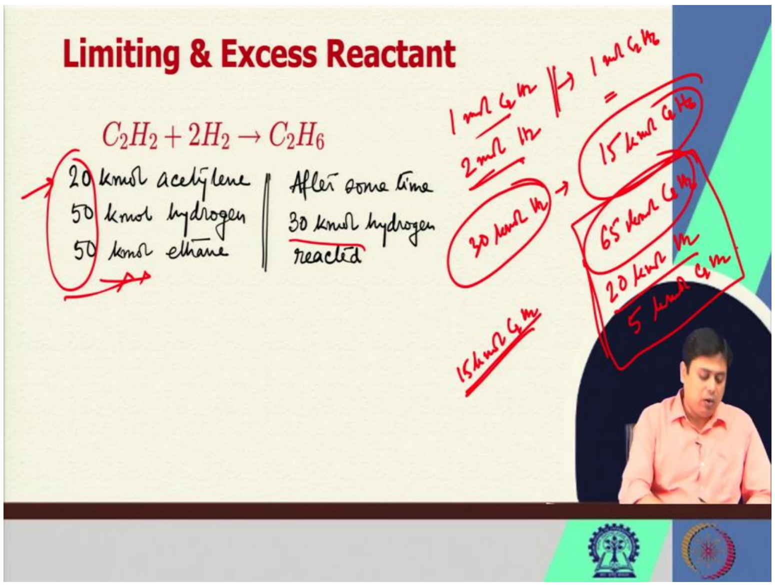

Now coming to the second part that is how do we calculate the molar composition of the product gas but before that I again go back to the problem statement that I started but we have not answered there because that time I mentioned we need to understand which is the what is the extent of reaction. Now say we take a pause here and we shift to a different reaction where we have number of species are lower so that we can easily understand.

So here the involved this species in the reactions are the acetylene hydrogen and ethane where this is the inlet feed condition and after some time we see that 30 kmol of hydrogen is reacted. So, what are here the product composition? What is the product composition in this case or what are the components of the product here that would come out. So, here we can see that one mole of C_2H_2 is reacting with 2 moles of H_2 in order to produce one mole of ethane.

2 moles of CO_2 reacts to form one mole of ethane. Now here after a certain time we have seen there is 30 kmol of hydrogen that has reacted. So, how much of C_2H_6 has been produced. So, we can understand that we have 15 kmol of C_2H_6 has been produced by 30 kmol of hydrogen at the same time in the feed itself there was 50kmol of ethane which means we have total 65 kmol of ethane in the product.

30kmol of hydrogen has reacted but 50k mol of hydrogen is fed. So, which means in the product stream we have 20 kmol of hydrogen that is unreacted we see that 2 moles of H_2 reacts with one mole of C_2H_2 to form the one mole of product. So, which means 30 kmol of H_2 when reacted it actually consumed 15 kmol of C_2H_2 the amount fed in the feed was 20 kmol of acetylene which means we have 5 kmol of C_2H_2 left in the product stream.

So, the product stream will have 65 kmol of acetylene 20 kmol of hydrogen and 5 kmol of acetylene this would be our product composition. So, the point here is that how do we generalize this formulation.

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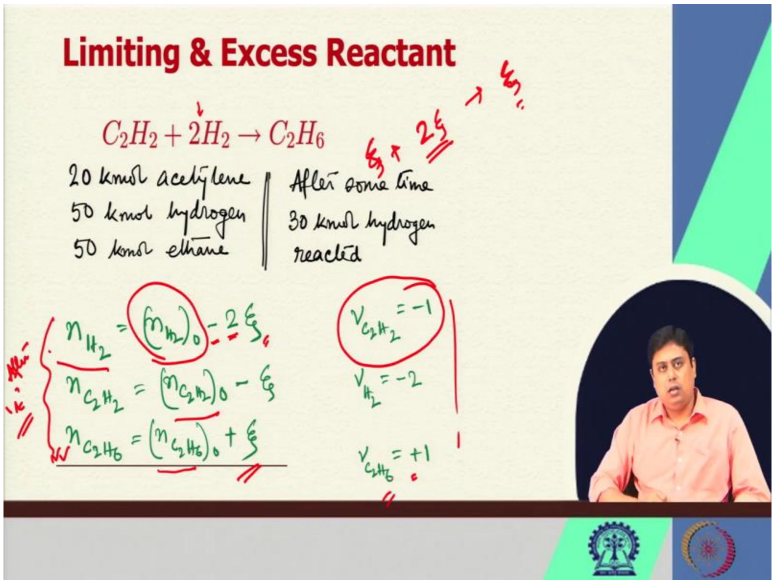

So, that we can apply it for any problem like the one that we have started for that we introduce a parameter ξ. So, the ξ is a parameter that has the same unit that is of either mole or molar flow rate depending on whether it is a batch system or a continuous process. So, by this, what we understand that 2ξ this amount, this is the amount that is being consumed in this case. So, 2ξ amount is being consumed in this case for ξ amount of C_2H_2 with C_2H_2 in order to produce 1ξ amount of C_2H_6.

So, that means after a certain time the amount it has converted the hydrogen that has been converted is mentioned by the extent that it has been converted that is the extent to which the reaction has happened. To quantify that here we can write that this is the initial or the feed condition that is the feed mole the amount of mole of hydrogen in the feed and since this is a reactant after a certain time the number of hydrogen mole would be lesser that is the subtraction we have the – sign for any reactant × its stoichiometric coefficient and ξ which is the extent of reaction.

So, this extent of reaction is multiplied with its stoichiometric coefficient in order to generalize a form. So, similarly for acetylene what we can write these are the amount after a certain time t. So, number of moles of acetylene would be its feed – the extent of reaction. Ethane which is the product here if that was there in the feed condition or if it is there in the feed + the extent of reaction × stoichiometric coefficient.

So, here this new we introduce as the stoichiometric coefficient because we are now trying to generalize this form for any reaction we will try to find out what is the product composition. Now the stoichiometric coefficient here that we mentioned here is the nu and to simplify the scenario or to correctly understand its importance we write negative sign when it is a reactant and positive sign when it is a product because reactants will be consumed products will be generated.

So, based on this we can write or we can identify that the stoichiometric coefficients are for acetylene – 1, for hydrogen – 2 and ethane it is + 1.

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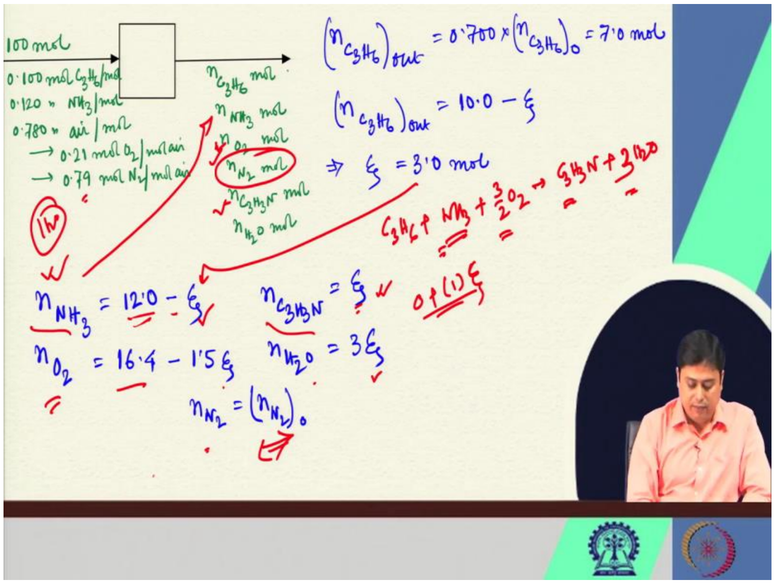

So, which means we can write a generic form for any species i in the feed stream or in the product stream as like this that is the number of moles of ith component at any time t is equal to its inlet amount or the input amount of that ith species the stoichiometric coefficient × extent of reaction. The extent of reaction for all the reactive species or other reactants and the products are identical.

The stoichiometric coefficient nu i its sign will depend whether it is a reactant or the product because if from this this generic form has been arrived. Now if you cross check it or if you look back from this expression to all the 3 you would realize that when i is hydrogen the $(n_i)_0$ is basically $(NH_2)_0$ the stoichiometric coefficient of hydrogen for this reaction is 2 but since it is a reactant we write that as – 2 × extent of reaction.

Now the utility of this extent of reaction is that if you know any of these values that is either the inlet composition or the composition at a time t or the outlet composition you can calculate the extent of reaction for that species. For ith species if you either know its inlet composition or the inlet amount or the input amount or the output amount in number of moles you can calculate extent of reaction for that species which is identical for all other species or all other reactants and the products.

And that is the typical case that happens that means in the problem that we were discussing we saw that there was inlet composition was mentioned. And this nu we can estimate or we can get this value from the balanced reaction or from the stoichiometry this is always known to us. And then what happens once these 2 components are known for a species we can easily calculate what is the extent of reaction?

And then we use this extent of reaction for calculating the other species that what would be its composition. So, if we now apply this concept to the problem that we are solving that we have 100 moles of feed that was the basis of calculation and we had 3 reactants that is the reaction was $C_3H_6 + NH_3 + 3 / 2\ O_2$ giving us $C_3H_3N + H_2O$ and we had to balance it, this was the reaction.

This is the reaction that I am talking about. So, in this case based on this understanding of extent of reaction what we can see at first that C_3H_6 we have identified as the limiting reactant and also we have realized that what is the conversion which is the 30% of the limiting reactant 30% has been reacted or it has been converted. So, the remaining is 70% and that remaining would come out as the product.

So, that means the out means the output of C_3H_6 would contain 70% of the inlet value or the input value. Now this was the 10 moles as the inlet feed composition we can see for this basis of calculation. So, which means 7 mole of C_3H_6 is going out of the system. Now the point that we just discussed based on the extent of reaction is n_i is the output mole, $(n_i)_0$ is the input mole, nu_i is the stoichiometric coefficient, and ξ is the extent of reaction we apply that concept here.

That means we have this output moles is equal to input moles which is 10 moles + the stoichiometric coefficient. The stoichiometric coefficient for this is 1 but it is a reactant. So, it is – 1 × the extent of reaction which is unknown here. This seven mole is basically that is coming out. So, which means we can easily calculate what is the extent of reaction. Now this extent of reaction is of now tremendous help because NH_3, O_2 the products we can now quickly write in this form because again the reaction was $3H_2O$.

So, we can see NH_3 input – ξ because – 1 is its stoichiometric coefficient minus for the reactant and one for the stoichiometric coefficient that we have is this. We replace it here we can calculate what is the number of moles of ammonia in the output stream or in the product stream this value. For oxygen this is the input – 1.5 × extent of reaction we replace this value we get this value.

The number of mole of C_3H_3N is just the extent of reaction because in the inlet there was no C_3H_3N. So, that part is zero. So, 0 + stoichiometric coefficient × ξ which is simply ξ that is written here. Similarly for H_2O we see that is 3ξ because water was not fed in the feed. So, we replace these values here we get all the n values. Now we must not forget that there is also nitrogen which is inert which is not participating in the reaction.

So, the amount that was in should come out as the n outlet which is we have here is the 78 × 0.79 moles of nitrogen. Once we have this we can get the total number of moles by adding all the n's and can find the mole percentage for the corresponding species. So, we stop here and as you have seen the glimpse of the next lecture we will understand what chemical equilibrium is in the next class.

And how we apply this concept of extent of reaction to the chemical equilibrium as well and how to find in those cases the product compositions. But remember these are the fundamentals and we have yet to apply all these knowledge for the material balance. So, these are the fundamentals and the introduction to this reaction stoichiometry. So, thank you for your attention and will see you in the next class with a new topic on the equilibrium, thank you for your attention.