Material and Energy Balance Computations
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Lecture –21
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 were studying multiple reactions its few terminology that are necessary for applying the balances on a reactive system or the processes.

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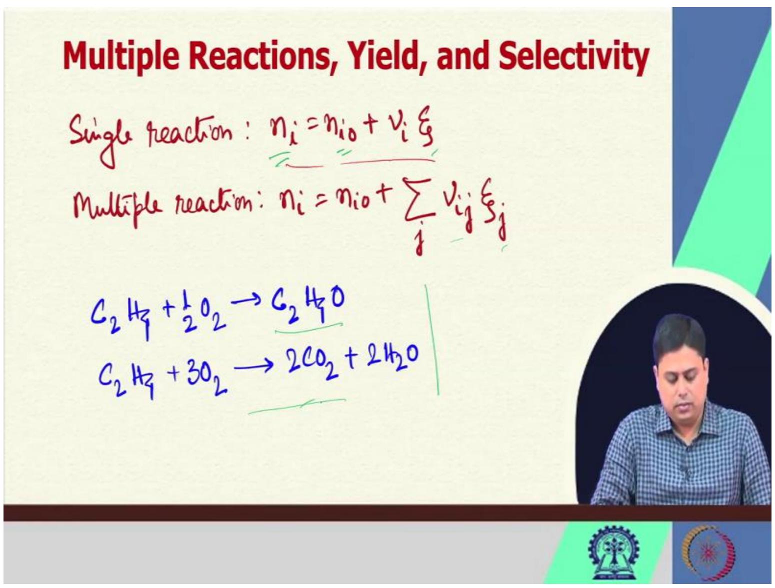

So, what we have seen earlier is the definition of yield, selectivity, percentage or fractional conversion. Now we started to know that whether the extent of reaction that we have understood and realized in the last class whether that can be extended for the multiple reactions or not. Now it is indeed we can apply that whatever we understood for the single reaction which is mentioned here the extent of reaction the concept of it that the number of moles or the molar flow rate at the outlet = the moles or the molar flow rate at the initial stage or at the inlet + the stoichiometric coefficient.

Now this stoichiometric coefficient is positive for the product, negative for the reactants and the extent of reaction. Now for multiple reactions the similar concept we can apply and in this case for each and every independent reaction. We have to assign one extent of reaction. So, if j is the number of reactions that is happening or that are happening in that case it is the summation of the stoichiometric coefficient of ith component in the in that particular jth reaction and the extent of reaction in that reaction.

So, say let us elaborate this with an example. So, in the last class we stopped here that I showed you these 2 reactions where ethylene is being oxidized and while doing so, ethylene oxide is produced as well as some carbon dioxide is produced. Now our desired product say ethylene oxide and this is the side reaction or extra reaction that is happening. Now how do we apply this concept for this multiple reactions.

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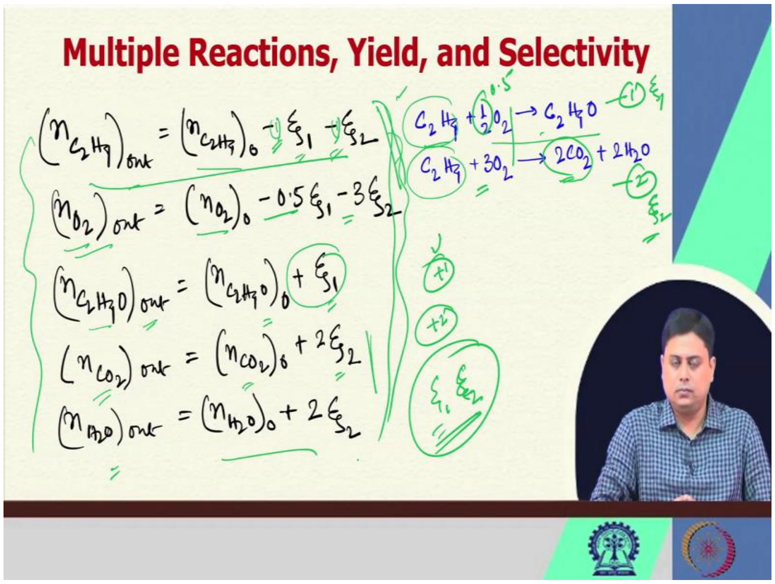

Say for this case if this is the set of reactions that we have what we can write we go step by step through each and every equation and we see that the components C_2H_4 the ethylene at the output = its mole, number of moles in the input. Now this is the reactant in both the cases. So, its stoichiometric coefficients in the first case it is – 1 in the second case it is also – 1. So, it is having the new values for first reaction it is – 1.

For the second reaction it is – 1 and the extent of reactions we assign here for the first reaction it is ξ_1 and for the second reaction it is ξ_2. This is how we apply the extent of reaction understanding to the multiple reactions. Now similarly for oxygen, now here if you look at it oxygen also is involved in both the reactions. So, its output compositions or output moles or the molar flow rate depending on the problem statement it would be the input value this is reactant.

So, again – sign with the stoichiometric coefficient for the first one it is half that is 0.5. So, – 0.5 in the second one it is 3 and again since it is a reactant we have – 3. So, these are the reactants. Now coming to the products one of the products is ethylene oxide which is at the output = its input + it is being produced in only one reaction. So, it has only one component additional in the right hand side which is + ξ_1 because here it is the product. So, the new value of it is the + one and the extent of reaction for the first one we defined as ξ_1 and in this case it is ξ_2. So, it is + ξ_1.

Similarly for carbon dioxide it is the input it is the product. So, the stoichiometric coefficient is + it is happening only in the second reaction. So, it is + 2 × the extent of reaction of that reaction which is ξ_2. Similarly water is being produced in the second reaction itself. So, like the carbon dioxide we can write the composition here in such a manner. So, which means we had here 5 species it all the concentrations or all the composition are now expressed in terms of extent of reactions which are specifically here ξ_1 and ξ_2 that means we have only 2 unknowns.

So if any 2 compositions any 2 species their moles or the molar flow rates are known at the output we can easily calculate then ξ_1 and ξ_2 because we have 2 unknowns. So, we need minimum 2 equations to solve that the unknowns once we find these values we replace it here to have the outlet composition of this system. Now this is important because when we apply for the reactive processes one of the way to apply or to solve such system is this extent of reaction we will further elaborate when we will do the example in those cases.

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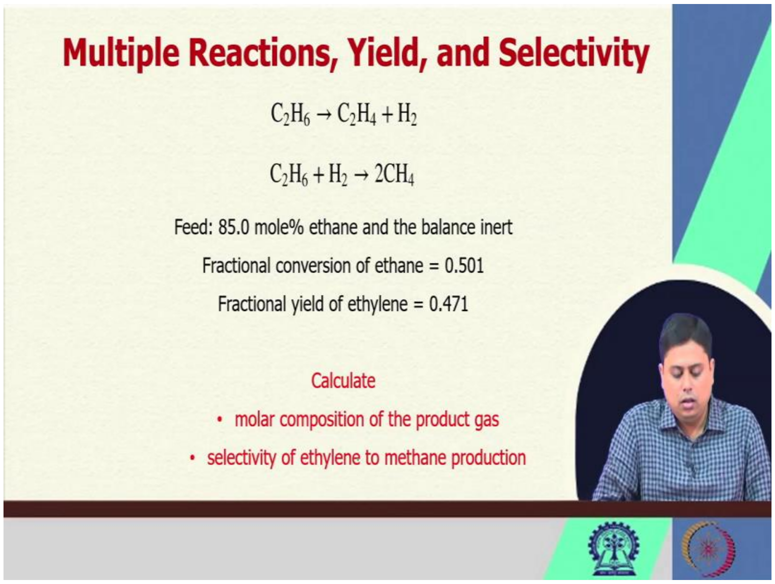

Now if we solve this problem this would give us more insights on what is basically say the selectivity and how do we actually calculate this extent of reactions. So, say here we have ethane and ethylene so from ethane we are producing ethylene and as soon as this happens it further creates methane. Now the feed consists of 85 mole percent ethane and balance inert. Fractional conversion of ethane is known to us.

Fractional yield of ethylene is also known to us. Our job is to calculate the molar composition of the product gas in the first part. Subsequently we also have to calculate or estimate the selectivity of ethylene with respect to methane production. Now if we recapitulate the fractional conversion and fractional yield the fractional conversion is the amount of the reactant is converted. The fraction of its converted with respect to the feed composition.

The fractional yield of ethylene is that the amount of ethylene being produced with respect to what could have been in an ideal scenario if there were no side reactions. So, based on this understanding let us say we solve this problem quickly.

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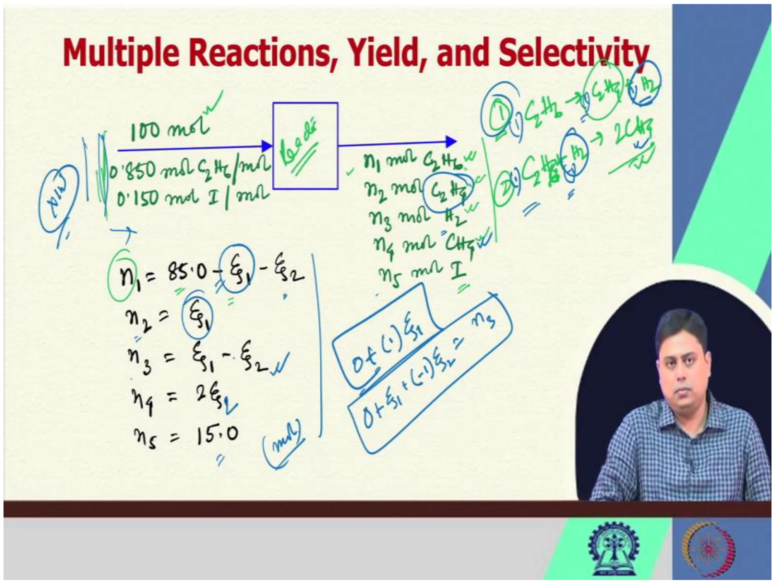

Now here our first task is to draw the flow sheet or the flow diagram. So, here what we have a reactant a reactor in which certain known composition of feed is coming in and the product is being formed. Since here the molar composition is mentioned it is logical to assume the basis of calculation as 100 mole. So, if the feed is of 100 mol there we have 85 mole of ethane and 15 mole of inert.

Now this is converted into some product which is ethylene that is the desired composition desired product and methane which is undesired product. Now since here fractional conversion is mentioned and fractional yield is mentioned which means not all the reactants have been converted to products that means there will be some unreacted reactants in the product. So that is why we have to be careful in writing the product stream the composition of it.

Now, since, there will be unreacted reactant and that is specifically ethane. So, here what we have the reaction is C_2H_6 giving us $C_2H_4 + H_2$ and as soon as that happens hydrogen is produced, it further creates methane. This is our desired product this is undesired product. So, we have unreacted reactant in the product stream of n_1 mole which is unknown we have product of n_2 mole, we have further hydrogen that is one of the products of the reaction.

We have methane and we must not forget about inert that will not take part in any reaction and will come from the output stream as it is or from the reactor as it is. So, now if we apply the extent of reaction concept here what we understand we have multiple reactions and specifically here we have 2 reactions. So in one, if we define this for amount of C_2H_6 then it is the input amount which is 85 moles.

This is based on the assumptions that we have 100 moles of feed. So, 85 – ξ_1 because if we consider this is the first reaction and this is the second reaction the extent of reaction in the first case it is given as this value from stoichiometry we can see that this has a stoichiometric coefficient 1 and since this is a reactant it is – 1. Similarly for equation 2 here also we have stoichiometric coefficient one and it is a reactant in that equation as well.

N_2 is the amount of ethylene which is formed in only one reaction that is equation number 1. So, this = extent of reaction of the first reaction because there is no ethylene in the input stream or at the inlet stream. So, it is zero + stoichiometric coefficient of one because it is a positive, it is positive because of it being a product × the extent of reaction of that reaction. Similarly for hydrogen, now hydrogen in the first reaction it is the product but in the second reaction it is the reactant.

In the input stream there was no hydrogen. So, it is 0 + because it is the product in the first reaction with the stoichiometric coefficient of 1 it is ξ_1 + the stoichiometric coefficient of – 1 because it is a reactant in the second reaction × its extent of reaction which is n_3 that is $\xi_1 - \xi_2 = n_3$, n_4 is methane, amount of methane that is produced only in second reaction. So, it is 2 ξ_2 and at the end we have n_5 which is 15 mole because it is not reacting with any species it is inert.

So, whatever comes in as inert that must go out which means n_5 = 15, this is all we have in moles. So, which means now we have a set of equations with 2 unknowns.

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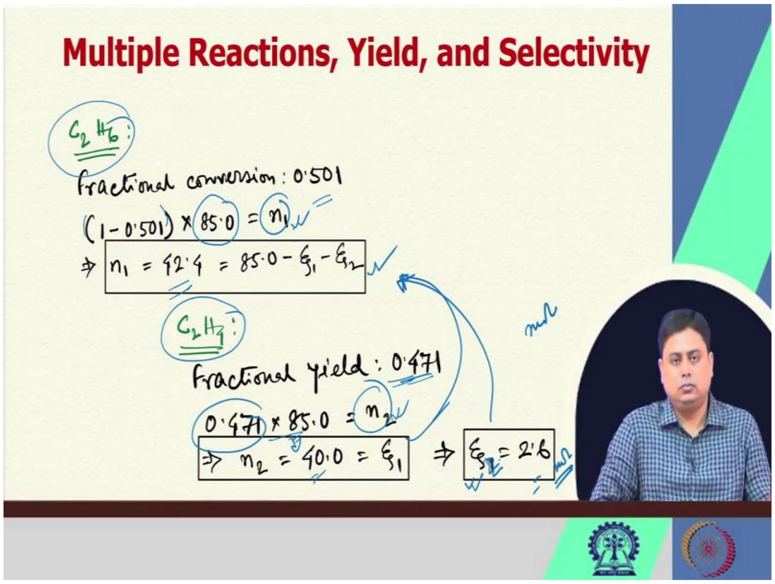

Now the information that is given in the system or in the problem statement is the fractional conversion. The fractional conversion the value is given as 0.501 that means the fraction of the feed amount that has been converted to the product. In the output stream that means some unreacted reactant is leaving. So, if this much fraction is the converted one the unconverted part is 1 – this value.

Now this unconverted fraction of the inlet value which is 85 moles of ethane if we look at the ethane balance in the input we had 85 moles of ethane and its unreacted amount is 1 – the fraction that has been converted which is 1 – 0.501 this is the n_1 which is in the output that the methane composition the number of moles of methane in the output. So, what we have n_1 = this value which is 42.4 and that = that we have written here $85 - \xi_1 - \xi_2$.

So, that means here we had 4 equations with 2 unknowns we had to know at least 2 of these values to calculate or to estimate the values ξ_1 and ξ_2 out of which we have just got 1 that n_1 value from the fractional conversion. The other information that is given is the fractional yield of ethylene. So, if we now look at the ethylene balance the information given is the fractional yield that is 0.471. So, this is the amount of ethylene being produced per or with respect to what could have been if there is an ideal situation and no side reactions were happening.

So, this fractional yield the fraction of its optimum production is happening with respect to its feed amount which is 85 moles based on the stoichiometry. So, here if you look at it, it shows that one mole of ethane in an ideal case without any side reaction can produce one mole of ethylene, clear. So, which means what we have if 85 moles is of ethane is there in the input stream it could have produced 85 moles of ethylene if there were no side reaction.

But it is happening only 0.471% fraction that is 47.1%. So, this × 85 in an ideal scenario is the fractional yield or that is in the product stream which is n_2. If you look at it n_2 is the product ethylene in the product stream. So, the fractional yield × the ideal amount that could have been if there were no side reaction of it in the conversion of ethylene that is the value of n_2.

So, this algebra comes out to be 40. So, n_2 value is now known to us, which is eventually ξ_1 from this equation. So, which means now we have 2 equations and 2 unknowns we can easily calculate, what is the value of ξ_2 in this case, because if we just replace it here we can get the value of the other component. So, that means we have ξ_1 and ξ_2 known to us where ξ_1 is 40 mole the units are the mole and ξ_2 is 2.6 mole.

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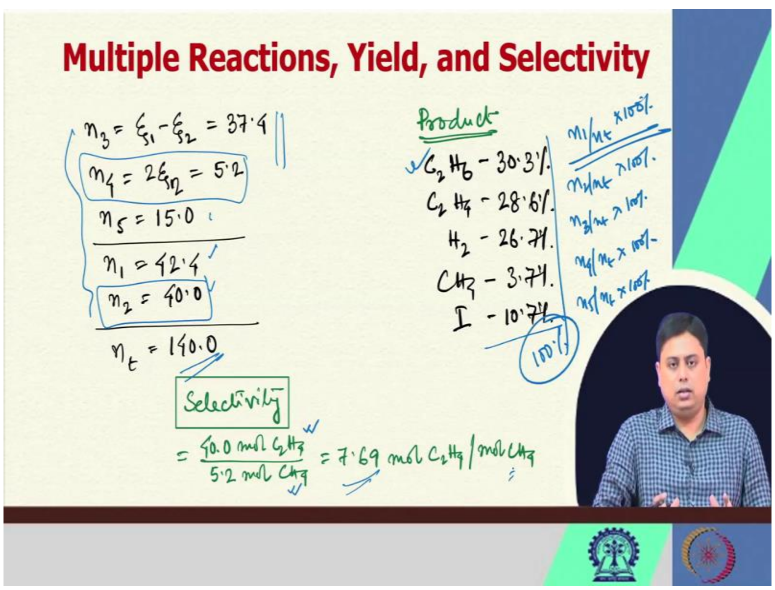

Once it is known we go back to this set of equations to find out the value of n_1, n_1 already we knew into n_1 we know. So, n_3, n_4 and n_5, n_5 is also known to us. So, 40 – 2.6 and 2 × 2.6 these are the values of n_3 and n_4, n_5 we knew n_1 and n_2 from which we have calculated ξ_1 and ξ_2. So, which means summation of all these ends n_1 to n_5 is 140 that means the product composition is now known to us which is n_1 / n_{total} × 100% for ethane.

For ethylene it is n_2 / n_{total} × 100% and similarly it goes on. So, we found the product composition to cross check if you add these all percentages it should be numerically close to 100% and here we see that it is indeed it is a 100%. Now the second part what is the selectivity of ethylene with respect to methane production because selectivity that has to be defined with respect to some undesired product. So, here the undesired products were hydrogen and methane.

Now here the question is with respect to methane. So, here we see that we have 40 moles of ethylene because n_2 this is the value in the output stream and methane is being produced as n_4 which is 5.2 moles. So, that means the selectivity is nearly 7.7 mole of ethylene per mole of methane. So, we have nearly 7.7 times of ethylene production than the methane production in this case that is the selectivity of this whole system or the whole reactive system.

So, I hope this part or this introductory section that is necessary for our reactive process balance or the reactive system balance is clear to you. So, in this part or in this introductory part what we have seen is the concept of yield, selectivity, percentage conversion or the fractional conversion and we have seen also the concept of extent of reaction.

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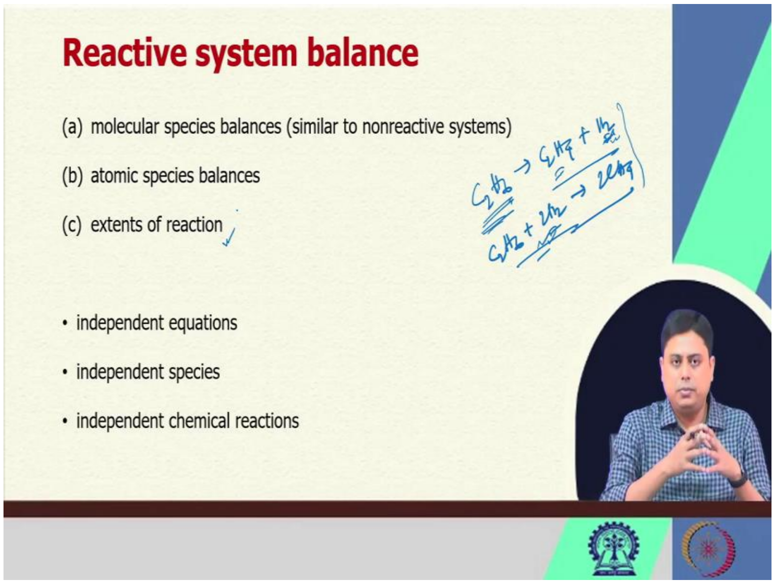

So now if we try to apply this knowledge for the reactive system balance in which we can solve the problem by 3 methods, one is the molecular species balance that is what we have done for the non-reactive system. But here the situation will be much more complex because each of the species that are involved in the reactions are either consumed or being generated. So, it is not further simple input = output, say for this reaction that we have just discussed ethane to ethylene production.

Now here the ethane the amount of ethane is fed to the system it is then consumed and ethylene is produced. Similarly in addition to this when we had the side reaction what we see that the hydrogen is produced in one case but in other case it is generated. So, it is not further the input is output it is the generation the consumption. If we consider such terminology it would be easier for us to identify. Because the molecular species here hydrogen is consumed in one case which is the second reaction and being produced in the first reaction.

So, molecular species balance in the case of multiple reactions in the reactive system is not straight forward but the atomic species balance because here instead of C_2H_6 some one can balance atomic hydrogen atomic carbon these are the 2 atomic species are involved in this whole reactive system. Now these atomic systems or the atomic species can neither be created nor be generated.

So, in such case the atomic species balance would eventually result like our previous simple way of solution that is input = output that is the atomic hydrogen that is given in the system it should come out in that amount at the atomic level. And then we can also apply the extents of reaction concept while solving this reactive system balance. But before going into these details in the next lecture we will start with a simple concept or the understanding of independent equation, independent species and independent chemical reactions.

So, we will take it off from here in the next class and we will see that how these 3 ways, the 3 methods that can be applied for a simple problem. And irrespective of the way that you take from these one of the 3's the result would be identical. Till then thank you for your attention.