**Basic Principles and Calculation in Chemical Engineering**
**Prof. S. K. Majumder**
**Department of Chemical Engineering**
**Indian Institute of Technology-Guwahati**

**Module-03**
**Lecture-09**
**Material Balances On Reactive Processes**

Welcome to massive open online course on basic principles and calculations in chemical engineering. So we are discussing about fundamentals of material balance with examples under module 3. In this lecture we will discuss that material balances on reactive processes.

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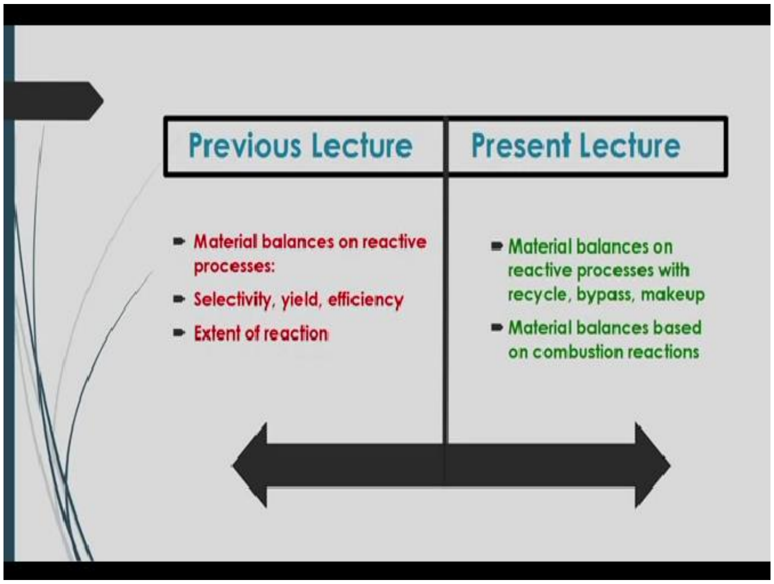


Here we have given earlier the examples of material balances with nonreactive processes like with recycle with bypass and by purge. Here we will discuss something more about that reaction processes like selectivity yield, extent of reactions and how this you know extent of reaction concept can be used to do the material balance on this reactive processes.

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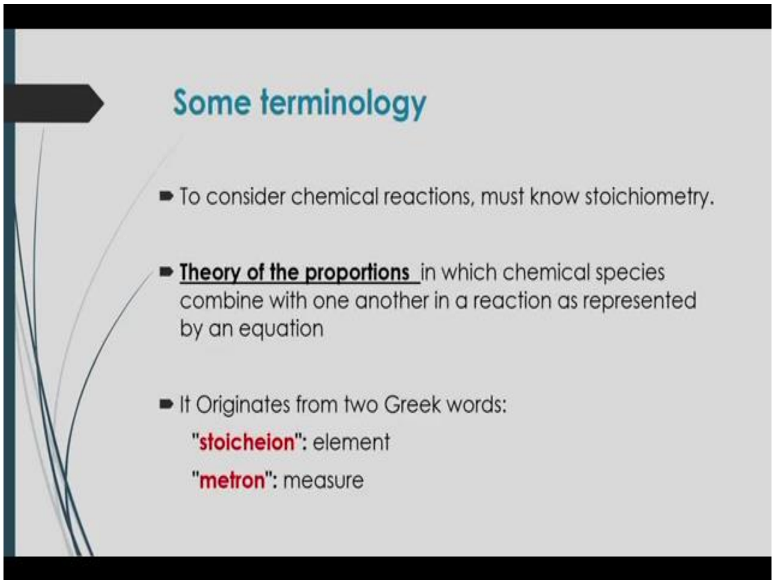


Now, before going to that calculation have to know some you know terminology of that reactive system . In this case to consider a chemical reactions, you have to know the stress immature of that reaction equation. Now, you know that theory of the proportions in which chemical species that combined with one another in a reaction as represented by an equation and that will be called as equation of reaction.

And did actually this you know that concept of this you know that reaction equation that is stoichiometry and it originates from two Greek words. That is, you know stoicheion that is called the element. And metron that is called measure. So, based on this stoichiometry is coming.

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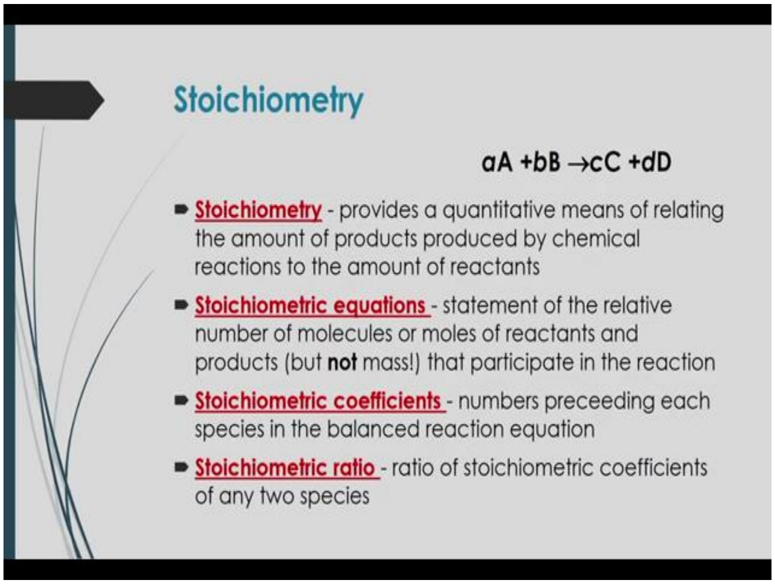

Now, this stoichiometry actually for a particular reaction equation, it will provide a quantitative means of relating the amount of products that are produced by chemical reactions to the amount of reactants. Whereas, in this stoichiometry you will see that to stoichiometry, you will get that the stoichiometry equation, that will give you the statement of the relative number of the molecules or moles of reactants and products.

But not mass you can say that participate in the reaction and the coefficients accurately represented by the numbers that will be proceeding a suspicious in the balanced in the reaction equation and stoichiometry ratio. This will be actually regarded as the ratio of stoichiometry coefficient of any 2 species. So, these are some you know terminology that you have to you know remember.

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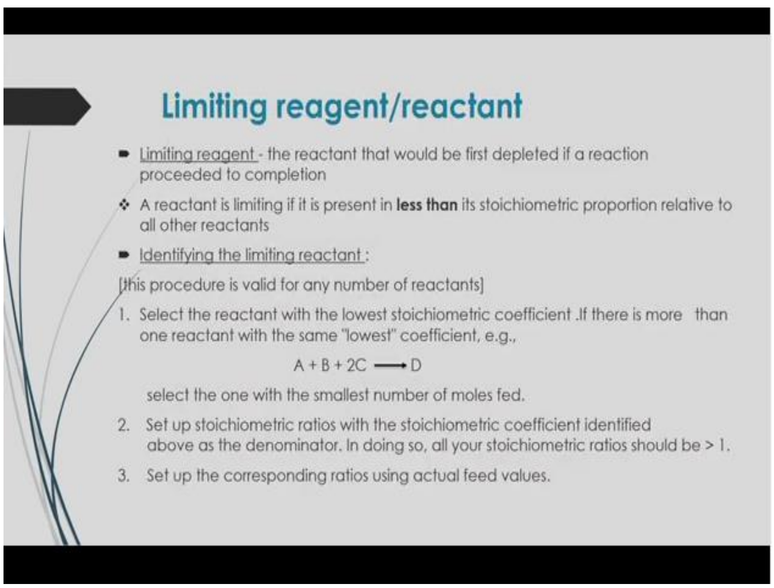


And you have to understand and also in reaction you will see some reactants will be you know, limiting reagent or reactant, in that case that reactant that would be first depleted if a reaction, you know proceed to combustion and proceed to completion. A reactant is limiting if it is present in less than it is a stoichiometry proportion relative to all other you know, reactants. Now, in this case you have to identify that limiting reactant.

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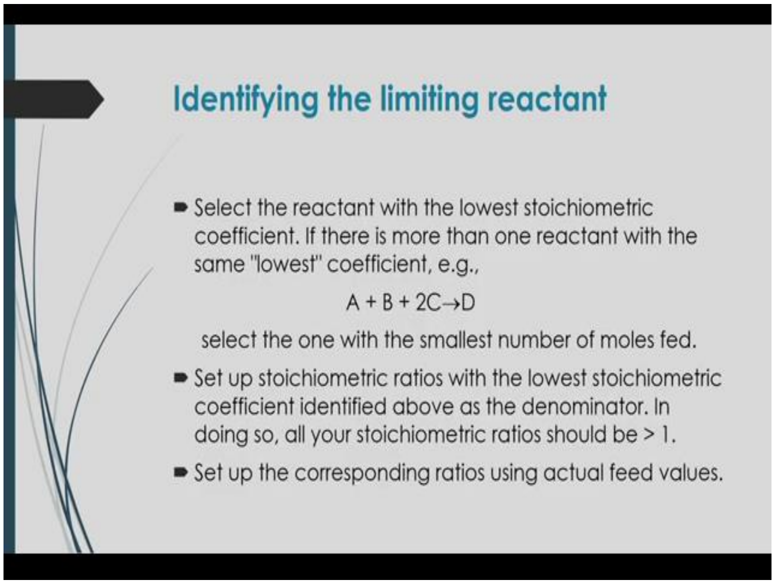


And now, how to that you know identify that limiting reactant there, first of all you have to select the reactant with the lowest stoichiometry efficient in a particular reaction. And if there is more than one reactant with the same lowest coefficient, example like this given here in this slides. So, in that case you have to select the one with the smallest number of moles fed. After that you have to set up the stoichiometry ratios with the lowest stoichiometry coefficient that will be identified as the denominator.

And in doing so all your stoichiometry ratios should be greater than 1, after that you have to set up the corresponding ratios using actual feed hallows. So, all these things you know earlier also because you have already completed all those things in you know schools levels also in high secondary schools, they are still you just go through this you know concept for your you know, understanding for what the calculation in the material balance.

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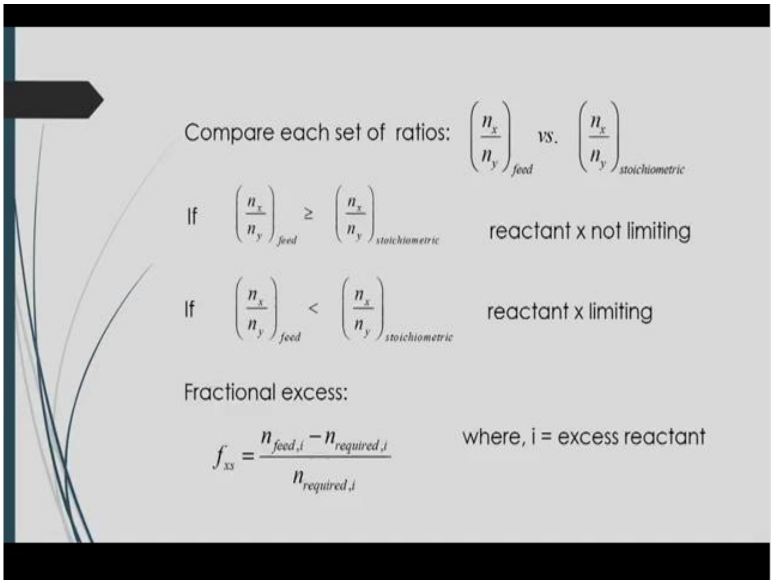


Now, in that case you will see that with that limiting reactant, how to actually find out that which one will be the limiting reactant. In that case, if you compare a set of ratios like here in x by n y that will be in the feed verses and an x and y that will be in the stoichiometry. So, if n x by n y in the feed is greater than equals to n x by n y in the stoichiometry coefficient, then you will see that react and x will not be limiting.

Whereas if n x by n y in the feed if it is less than n x by n y in the stoichiometry coefficient then you will say that x will be limiting reactant, other terms like fractional access sometimes you will see that to complete the reaction you have to supply some excess you know reacting to the that based on this it is limiting reactant and also sometimes the what will be amount of you know reacting to be supplied in the feed.

You have to you know calculate what should be the actual amount of reactant amount is required for your complete reaction theoretically and after that you have to you know judge of what should be the you know excess amount of that reactant is present in your you know feed mixer or if it is short is then you have to supply excess amount of you know that reacts in the feed mixer. So, that that you reaction will be completed.

Now, in that case you have to you know assess that you know concept of that you know excess reactant based on this you know fractional access equation here. So, in that case fractional access will be calculated as here f xs that will be equal to what will be the number of feet of that species i and also what will be the number of moles of i, but that is required for your complete combustion that you have to calculate.

And after that, if you divide it this you know that difference of that, you know, species are present in feed and presses are required for your complete you know reaction theoretically, if you make a ration then it will be called as that fractional access where i will be the excess reactant here in this you know reaction in this in this equation.

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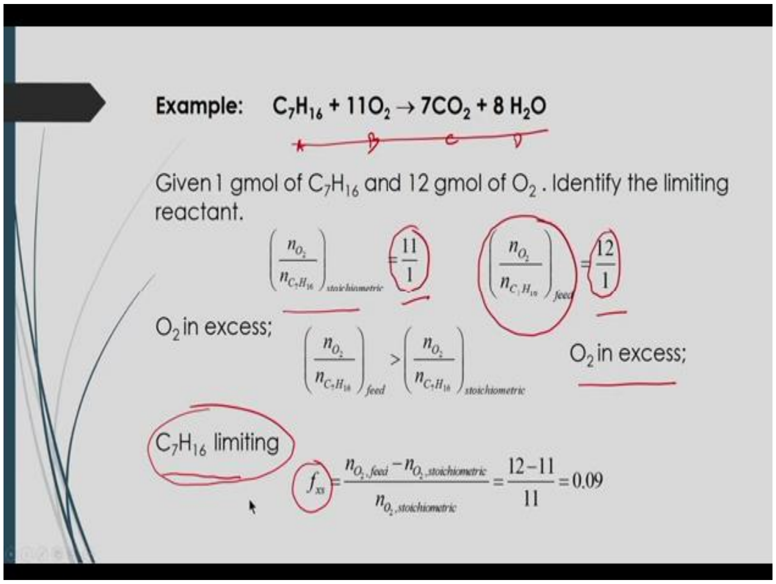


Now, if we consider an example of you know reaction like this here, it is given in the slides in this case see here A is reacting with B and gives you that C and D , in this case here coefficient stoichiometry efficiencies are 1 11 7 8 respectively. Now, in this case, given 1 mole of C 7 H 16 and 12 you know mole of oxygen. In this case you have to identify what the limiting reactant.

Now you have to find out first what should be the ratio of that oxygen 2 you know, here happen in the you know reaction then as per stoichiometry you know coefficient this ratio will be coming as 11 by 1. Whereas the ratio of these molecules in the feed to be 12 by 1. Now, it is simply that this 11 by 1 is you know less than 12 by 1. So, we can say that oxygen in excess air. So, oxygen is excess air.

So, we can see that oxygen in but excess but the limiting will be that other one that is C 7 H 16 here, because in this case you will see that this C 7 if we compare that it will be you know less than that feed. So, accordingly we can say that this C 7 H 16 is limiting and what is the you know fraction of excess of that you know excess of that limiting reactant, here as part that equation earlier given here like this accordingly you can get what should be the excess of that limiting reactant. So, this will be your 0.09 in this case.

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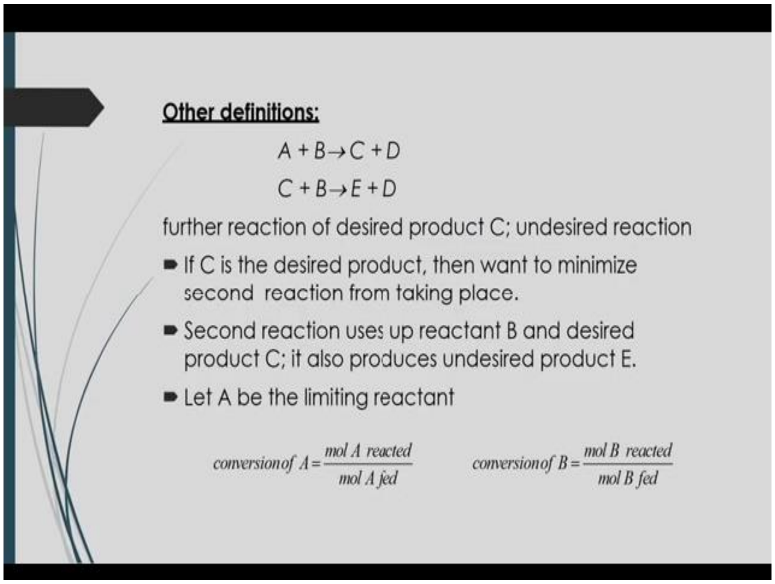


Other definitions like suppose there are 2 reactions A + B which will give you C and D and C + B which will give you E and D. Now, further the reaction of desire products C, and is that reaction will be there in particular set of reactions. Now, in this case if C is a desire product then you have to minimize the second reaction from taking place. And also second reaction uses up react B and desire production C.

It also produces undesired product, let A be the limiting reactant here, so conversion of A = mole of a reacted by mole of A fed and conversion of B will be represented by mole of B reacted by mole of B fed.

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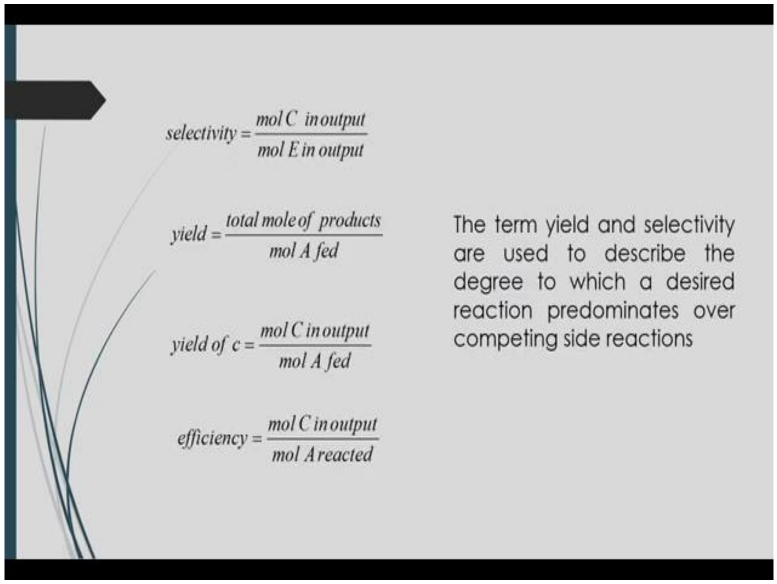


And you can select that which component to be you know that desirable or undesirable based on that selectivity. So, that selectivity will be you know defined as mole of C in output by mole of E in output as far you know that reaction and yield will be defined as here, this total mole of products by total mole of A fed and yield of C for particular species, then you can say that mole of C in output by mole of A fed.

And efficiency of the you know that you know productive output of C will be equal to mole of C in output by mole of A reacted. Now, in this case, the term yield and selectivity are used to describe the degree to which is a desired reaction predominance over competing side reaction.

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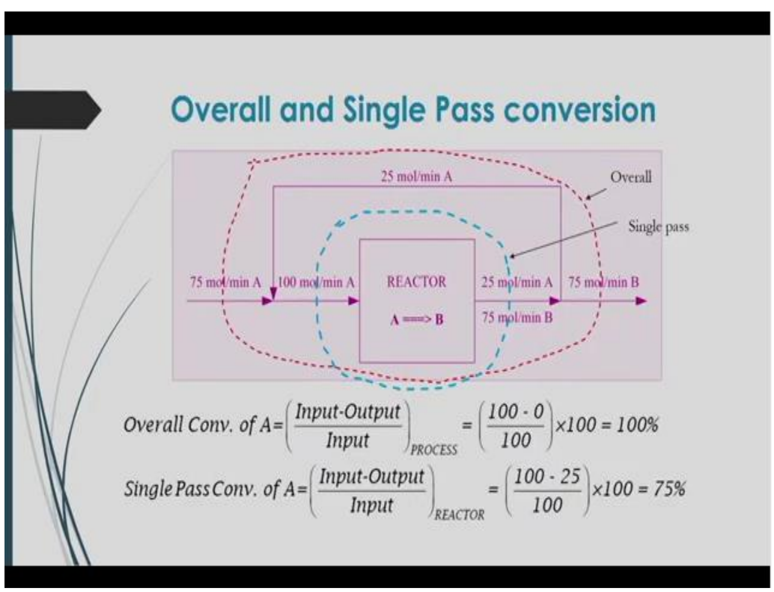

And other important you know terminology that you have to you know remember sometimes it will be required for your you know material balance calculation based on a reactive system. Now, in this case, if we consider that certain process you need a reactor where the reaction is going on and A will be giving to B in that case A is coming at a certain flow rate after mixing with it is recycle here.

And it enters to the reactor at a certain rate and after that reaction, it will give you the you know mixture of you know unreacted A and the product B and there will be certain flow rate of that A and B and after that it will be coming out and to be separated in a certain process unit and then has a product you will see that some amount of you know product that will be here. It will be you know taken but remaining you know unreacted you know that reacting to be you know saying back to each you know, mixer before you know processing the top reactive there.

So, here in this case one interesting term that you have to know that overall conversion of the A, how you define it. Now, for overall conversion of A you have to consider that whole process here, whole process means including that mixer, reactor and separator. So, in that case this overall conversion of the A would be represented by what should the input of A and what should be the output A output of A there and divided by input of A.

So, here you will see that input is coming as 100 mole per minute, whereas output is you know that there will be 0 for specifically for component A. So here 100 – 0 by 100 that will be into 100 and that means here to be 100% overall conversion. Whereas, if you are considering that there will be a single pass conversion that means here what would be the input of A in a particular process unit like here reactor.

That case only you have to consider here the reactor. So, for the reactor what is the input of A and for the reactor what will be the output of A. So, in this particular example, you will see that the input of reactor for this component A is 100 whereas output of component of this A only for this reactor it will be only 25 as shown here in the figure in the slide. So, you can calculate that single pass conversion of A will be equal to 100 minus this 25 divided by that 100 that means input.

So input minus output divided by input that will be regarded as single pass conversion of here particular species. So, here it is coming 75%. So, what is comparison that overall conversion and single pass conversion will be totally different. Overall conversion as far as here it is coming 100% whereas single conversion rate is coming 75%. So, this sometimes so this concept will be sometimes required for your you know material balance calculation in the reactive system.

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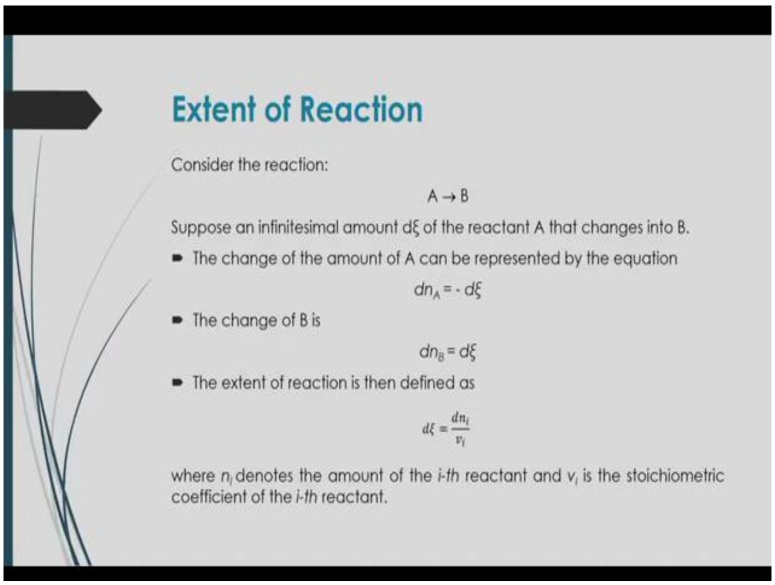


Now, another important aspect of you know reactive system that actually sometimes at a particular time what will be the amount of you know reactant is present in the system and what will be the you know reactant conversion and after conversion what to be the amount of reactant to be present in the you know system that also you know represented by certain you know concept is called extent of reaction.

Now, consider the reaction A which will give you a product B. So, in this case, if you assume that infinitesimal amount of you know de xi here 1 xi is considered here some this xi amount of you know that reactant A that changes into B. So, you are considered event some amount of A is converting to B that some amount of you know reactant will be denoted by this d xi. Now, this change of this amount of A can be represented by the equation here.

This dn A = - d xi, the change of B similarly, can be expressed as dn B = d xi because same amount of A will give you that you know product B here. So, dn B d xi. Now, similar to the extent of reaction is then defined as di xi will be equal to what will be the change of that component i, now with respect to you know it is a stoichiometry coefficient that will be divided by you know here nu i.

Here n i denotes the amount of i – th reactant and here nu i is the stoichiometry coefficient of the i th reactant So, in this way you can define that extent of reaction.

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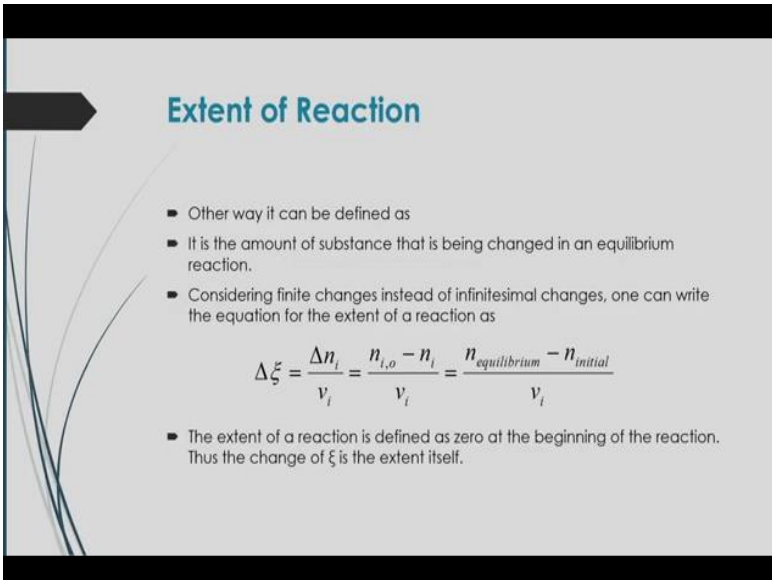


And other way it can be defined as like, it is the amount of substance that is being changed in an equilibrium reaction. Considering that finite changes instead of in finite simple changes on can write the equation for the extent of reaction as delta xi that will be equal to delta n i by nu i, then, it can be written as n i 0 – n i by nu i.

So, here in i 0 that may be you know that equilibrium power concentration that is at the outlet or at a certain time when it will be coming as equilibrium that equilibrium you know most will be there in. And initially moles will be in i initial you can say that and divided by stoichiometry efficient. So, in this way you can define that extent of reaction. The extent of reaction is defined as 0 at the beginning of the reaction because that is the changes of xi is the you know extent itself there.

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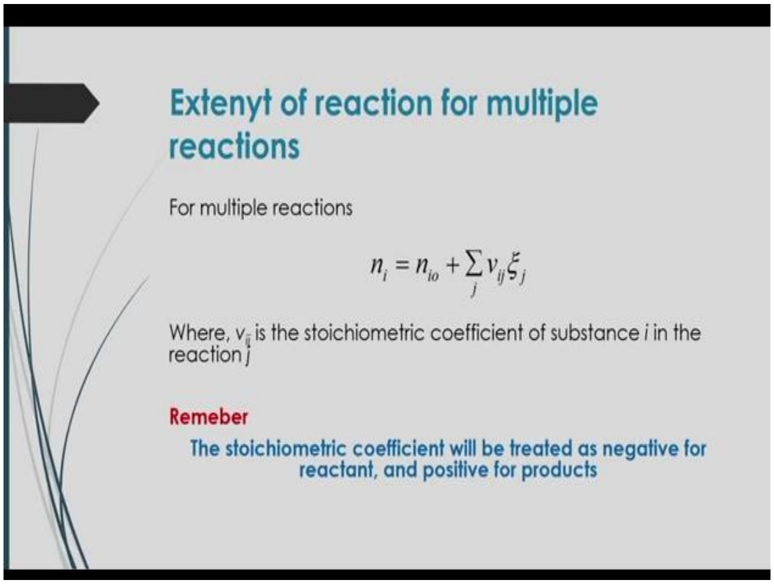


Now, you know that extent of reaction multiple reaction, how to you know calculate that, that case that for multiple reactions, this extent of reaction based on which you can you know, derive this equation as n i that means at a particular time what should be the moles of i present in that you know process unit that will be equal to n i 0 that means what will be the amount of i fed you know in the feed mixer.

And what will be that you know for summation of v ij nu ij into xi j. So, nu ij here stoichiometry coefficient of the reaction here j if there is j number of reactions are there, then you have to consider that nu i for particular reaction and similarly the extent of reaction for that reaction j will be denoted by xi j. So, accordingly this equation will be used for you know that extent of reaction calculation for a particular reaction.

Now, in this case interesting that you have to remember the stoichiometry coefficient will be treated as a negative for the reactant and positive for the product that you have to remember.

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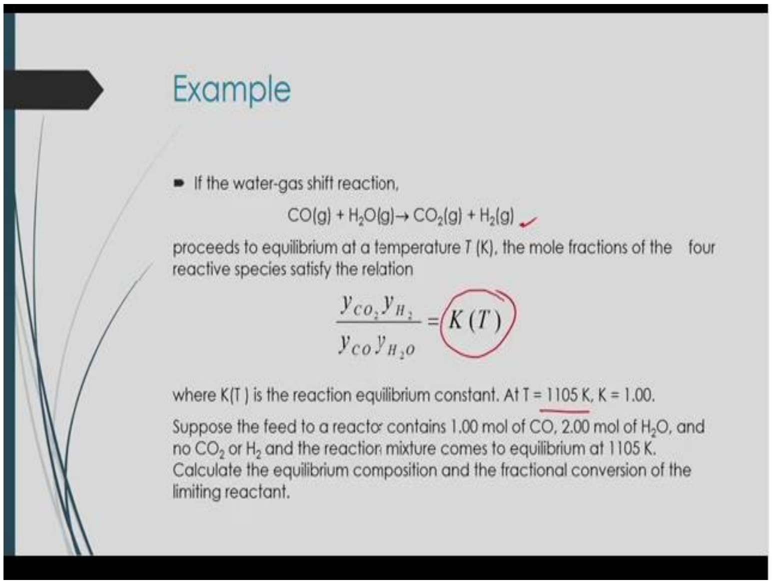


Now, let us have an example for this. Now, if water gas shift reactor like carbon monoxide plus water will give you that carbon dioxide and hydrogen gas, that will proceed to equilibrium at a temperature T Kelvin. Now, the mole fraction of the you know for reactive species to satisfy the relation here is given y carbon dioxide into y hydrogen divided by y carbon monoxide into water that will be is equal to some equilibrium constant.

Now, this you know equilibrium constant it is regarded as the reaction equilibrium constant at time that is 1105 Kelvin this K will be is equal to 1, now at this condition suppose the feet to a reactor contains 1 mole of carbon monoxide 2 mole of water and you know no carbon dioxide or hydrogen and the reaction mixer comes to equilibrium at 1105 K. So, in this you know operating condition of this reactor you have to calculate the equilibrium composition and fractional conversion of the limiting reactant.

So, here this y co 2 is represented by you know mole fraction of carbon dioxide and y H2 is mole fraction of hydrogen y co it is you know mole fraction of carbon monoxide and y H 2 o is simply that mole fraction of you know water. So, based on these at equilibrium condition what should we that equilibrium concentration of these carbon monoxide water you know carbon dioxide and hydrogen that you have to find out. So, you have to use that concept of extent of reaction here.

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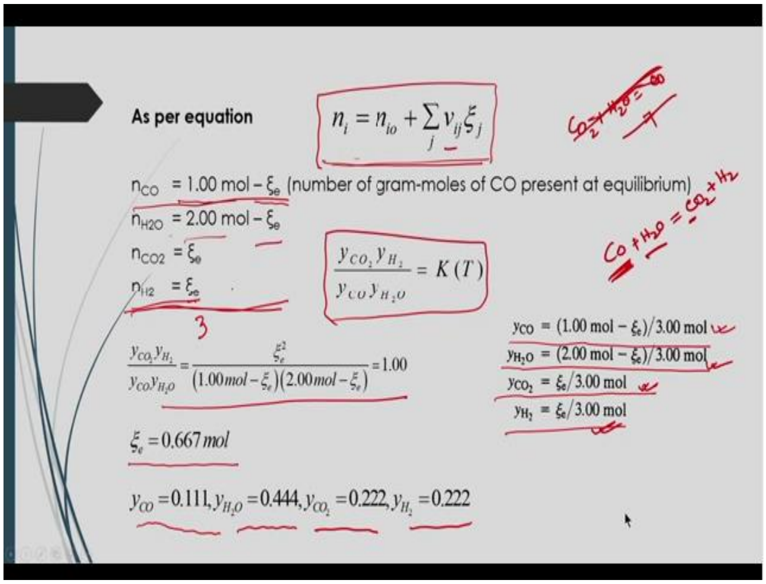


Now, let us solve this problem here as per equation we know that since here only one you know equation here. So, if we apply this general equation for multiple reaction, here in this case j will be equal to 1 only. So, n i = n i 0 + summation of nu ij into xi j her j only 1 that is one reaction is there. So, in this case, if I consider only for carbon monoxide first then here ni that means here n carbon monoxide that will be equal to what that what to be the feed amount of carbon monoxide this 1 mole whereas at equilibrium condition that extent of reaction will be able to xi i.

Now, in this case here as per reaction here what is the reaction equation is given carbon monoxide here, this is Co 2 + water that will be giving you what is that carbon monoxide as carbon dioxide here sorry, this is Co + sorry, Co + water that will be equal to co2 + hydrogen. So, this is your reaction. So, in this case you will see that if we consider that carbon monoxide, so, in the feed this amount of carbon monoxide is here 1.00 mole.

And here we can say that at equilibrium condition this extent of reaction is xi e. So, here for xi e we have to you know that considered this nu here as you know – 1 because this is reactant as we told that for the reactant this suckerfish and to be considered as negative whereas, product or consideration will be you know positive. So, here in this case this carbon monoxide it will be then represented by this equation here n co = 1 – xi e.

Similarly for water again you can consider here this coefficient is I think we are H 2 o here, this feed amount is here 2 moles is supplied in the feed, then n H 2 o = 2 – xi e, again here this coefficient is 1. So, it will be negative of 1 then it will be - 1 xi e. Similarly, for carbon dioxide if we represent it to be only here xi e, here in this case coefficient is 1 that will be positive since it is a product.

But here since there is no amount is supplied in the feed mixer. So in i 0 = 0 here, whereas, similarly for hydrogen it will be represented as xi e. Now, after that you have to you know calculate what will be the fraction in terms of this xi. Now, what would be the total you know amount of moles that first you have to calculate that you have to sum it up all those things and then you have to divide individual moles with that total moles then you will get that concentration.

So, here like this, if you sum it up this whole moles here you will get here simply 3 moles only. So, this is total mole is 3 moles. Now, then y carbon monoxide will be represented by this and similarly, y hydrogen will be like this and y carbon dioxide will be like this and y hydrogen will be like this, because this is simply mole fraction. Now, after substitution of mole fraction of all these components carbon monoxide, water, carbon dioxide and hydrogen you will see that this you know that in this equilibrium equation.

Then you can have this you know final form of equation after simplification and then after solving you will see that xi e = 0.667. So, this is called extent of reaction at its equilibrium condition. Now after the substitution of xi here again in this you know mole fraction of each component you will see that this mole fraction of component carbon monoxide it will be coming as 0.111 and mole fraction of water it will be coming at 0.444.

Here just substituting the value of xi i, similarly, for mole fraction of carbon dioxide you will get up the substitution of xi here and then hydrogen for hydrogen you will get this you know that the substitution of here So, finally, you can get these small fraction of carbon-di-oxide as 0.22 and hydrogen will be able to again 0.222. So, these examples will give you how to calculate that composition of you know that components in the mixer when it will be you know, as part a certain reaction with each, you know, output or products at a certain equilibrium condition.

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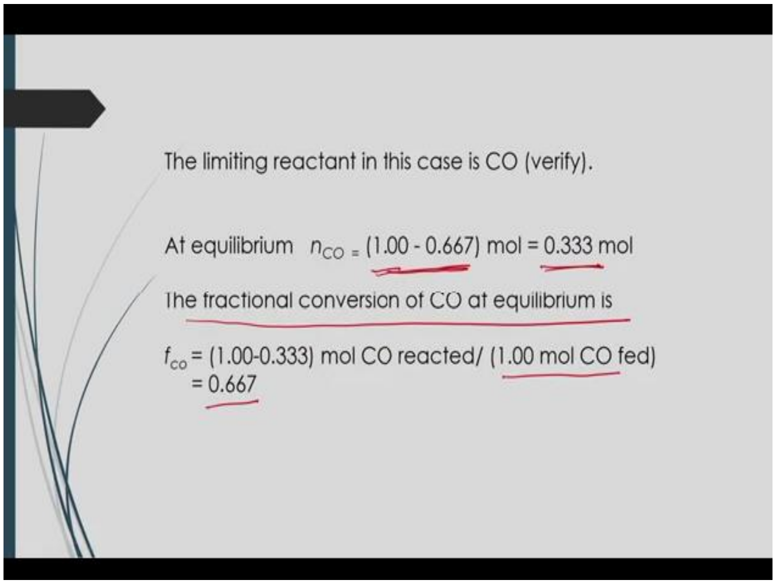


Now, what should be the limiting reactant in this case, you know that if you verify that principle based on earlier equation that I have discussed. So, it will be you know that the carbon monoxide will be as you know limiting reactant. Now, at that equilibrium condition what should be the you know carbon monoxide moles that can be calculated here that is what is the feed mixer and what to be the you know equilibrium mixer concentration.

So, it will be here simply you can say that that n co moles in the nu moles it is given your what is that 1 mole whereas, at the equilibrium condition it is coming 0.66 mole. So, based on that you can see that here it will be at equilibrium condition to be 0.33 mole and then fractional conversion of carbon monoxide and equilibrium will be as f co that will be equal to 1 - 0.33 mole, carbon monoxide that will be reacted divided by that 1 mole of carbon monoxide fed. So, it will be coming as 0.667.

So, this is your factional conversion of carbon monoxide. So, we can easily calculate based on that extent of reaction concept, what should be the fractional conversion of carbon monoxide and what really they are you know equilibrium composition in the mixer.

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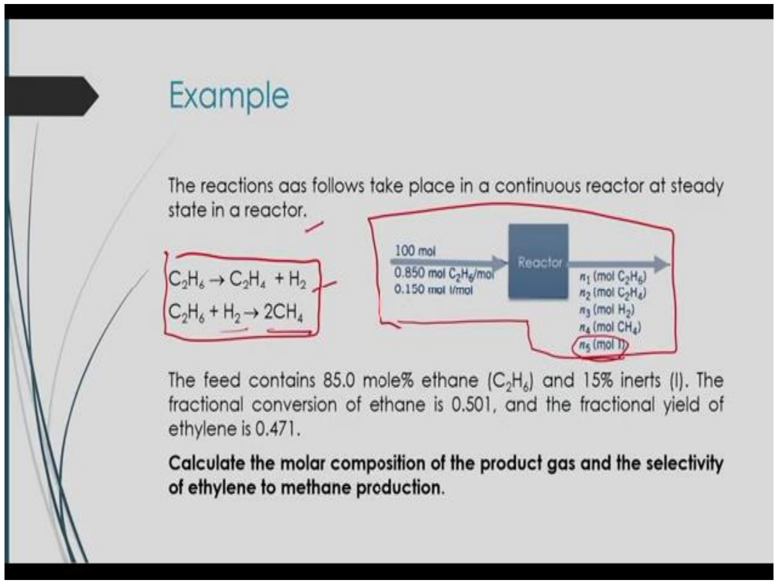


Let us do another example of this multiple with multiple reactions. In this case, if we consider that reactions as follows take place in you know a continuous you know reactor at steady state condition in a reactor. So, we can say that yeah this is one reaction that we see are ethylene, ethylene is given that, you know by this you know that by this conversion of you know ethylene. So, ethyl is actually obtained by you know conversion of you know ethane.

So, it is sorry ethylene is obtained from the conversion of you know that ethane at a certain temperature and pressure and also it will give you the hydrogen and then also you can see that this you know that ethane again reacting with that you know products hydrogen will give you that you know a methane. So, in this way based on this you know multiple reactions, how to calculate that you know that molar composition of the product cash and the selectivity of the ethylene into methane production that too can actually obtained by that concept of you know extent of reaction.

So, let us have these you know reactions that is going on in a reactor and you know that and the feed contains you know 85% ethane and 15% inerts and a fictional conversion of ethane is given 0.501 and the fractional of the yield of the ethylene is given is 0.471. So, as part this you know, schematic diagram here are closer to you can see that means here if we consider that 100 mole of mixer is going into the reactor out of is that 8.85 moles you know per mole of a feet, it is that means here 85% mole.

Then and you know 15% only inerts are going into the reactor and after reaction happens you will see them some you know methane then some amount of ethylene some moment of hydrogen, some amount of methane along with inerts to come in you know outlet stream such a product. Now, in this case very interesting that this is inert you know components will not take place in the reaction.

So, whatever amount of inerts will be you know going to into the reactor, that amount will be coming as you know in the outlet streams. So, that should be considered.

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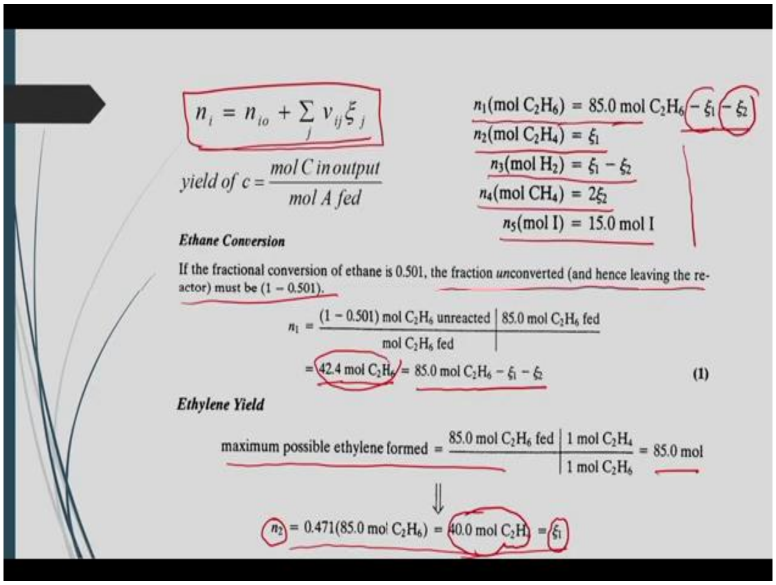


So, if I use that concept of that extent of reaction for the multiple reaction then this is your governing equation based on this equation you have to calculate all these things. Now, let us consider that n 1 according to this year, you know that flow chart n 1 is for you know C 2 H 6 that means, ethane n 2 power ethylene and what is that n 3 for hydrogen n 4 for methane and n 5 for inert amount in the outlet streams.

So, in that case if I use this, you know this extent of reaction equation here. So, n 1 can be represented by this here, but the feed amount is it 85 mole whereas as for this summation of P nu ij into the ij. So, if you substitute that the coefficient is you know 1 since it is you know that in the you know, reactant stream then coefficient will be negative. Similarly, the first reaction it will be a negative of 1 to xi 1 and similarly for the second reaction it will be negative of xi 2.

Similarly, for n 2 you can represent it as n 2 = x 1 since it is a product, then you have to represent this coefficient eta as sorry nu as positive terms. So, it will be positive 1 xi 1 here as part of equation similarly n 3 = x 1 – x 2 and n 4 = 2 xi 2 and n 5 = this 15 moles since it is not you know taking part in that the reaction and the same amount of energy inerts will be coming into the outlet to stream as what it is given in your inlet stream.

So, based on this concept of extent of reactions, we are getting this n 1 into n 3 n 4 and n 5 ethane conversion if we consider that, if the factional conversion of the ethane is 0.501 it is given in your problem, the fraction unconverted and hence, living the reactor must be 1 - 0.501. So, finally, you can calculate what should be the n 1. So n 1 will be coming as simply up to 42.4 mole C 2 H 2. Now, this n 1 actually as for that extent of reaction this simply 85 – xi 1 – x2.

Similarly ethane yield will be actually represented by the this equation it will be coming as 85 moles as by definition, then n 2 will be actually defined as like this, this one 0.471 into 85 then that will be is equal to as far as extent of reaction, we are no concept and 40 mole of that means, here ethane that will be equal xi 1. So, finally, you can get that this x1 will be is equal to here simply n 2.

That is among what is the amount here that will be 40 mole of you know ethane there, so xi 1 we have calculated and it will be as what is that n 2 and this is this amount is 40.

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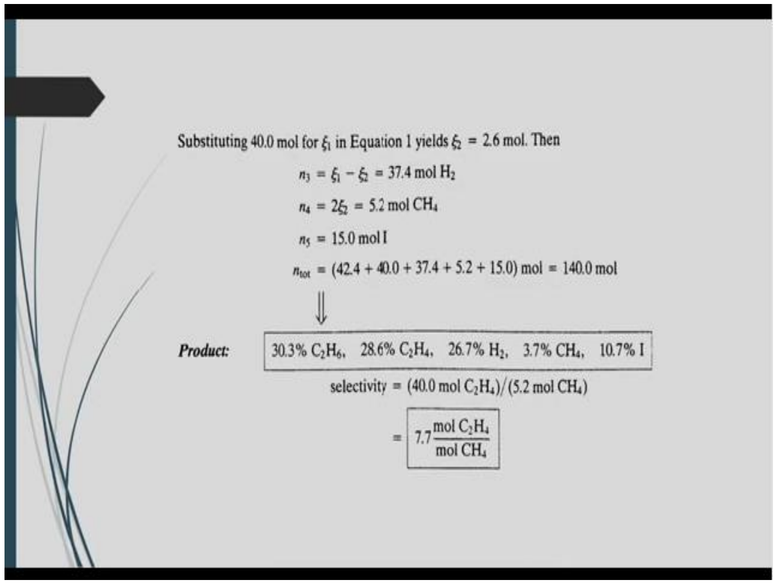


So, substitute on substituting this 40 mole for xi 1 in equation number 1 here given h. So, we can get that what will be the value of xi 2 there. So xi 2 = 2.6 mole. Then, after substitution of xi 1 and xi 2 in n3 then you can get that here in n 3 n 3 is basically x 1 – x2. So, after you know subtraction of x 2 from x1 you can get this n 3 as 37.4. Similarly, n 4 you can calculate like this to xi 2.

Xi 2 you know, so it will becoming 5.2 whereas n 5 is already known to you and then total mole will be is equal to see that will be summation of all the you know in n1 n2 n3 and n 4 and n 5 in the outlet steam, it will be coming as you know total amount 140 mole. So, after that you can easily calculate what from the fraction of all those components there. So, it will be simply individual amount of that you know component divided by total mole then you will get that by you know fraction of that you know, individual components.

So, it will be coming as 30.34 you know ethane 28.6 per ethylene and you know that 26.7% for hydrogen and 3.7% for methane and remaining 10.7% for you know inert in the outlet steam and based on these you can calculate what will be selectivity, that selectivity is defined as what to be the mole of you know ethylene produced based on what will be the amount of you know that methane by product is produced there.

So, this is simply 40 by here 5.2 then it is coming 7.7 mole of you know, ethylene in based on that total mole of you know methane in the outlet stream. So, this is the concept also how to calculate that selectivity and also what the mole fraction of our different you know, components are in the outlet streams based on the multiple reaction. So, please go through this you know examples and practice it. And then you will be able to solve other different problems based on that multiple reactions.

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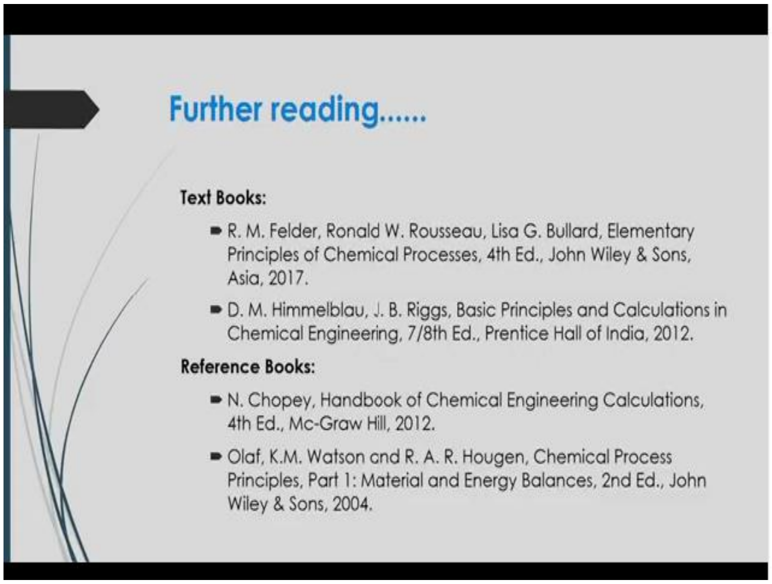


So, I would suggest you to follow this you know concept of that extent of reactions in these books like you know first textbook Felder, and Rousseau, and the elementary principles of chemical process 4th edition, you will get more information about this extent of reaction there and please practice some example problems given they are also. So, thank you. So, next lecture will try to you know describe more material balance based on you know reactive system even with multiple you know you need to recycle bypassed and you can make up and also some combustion reactions how to do the material balance on them, thank you.