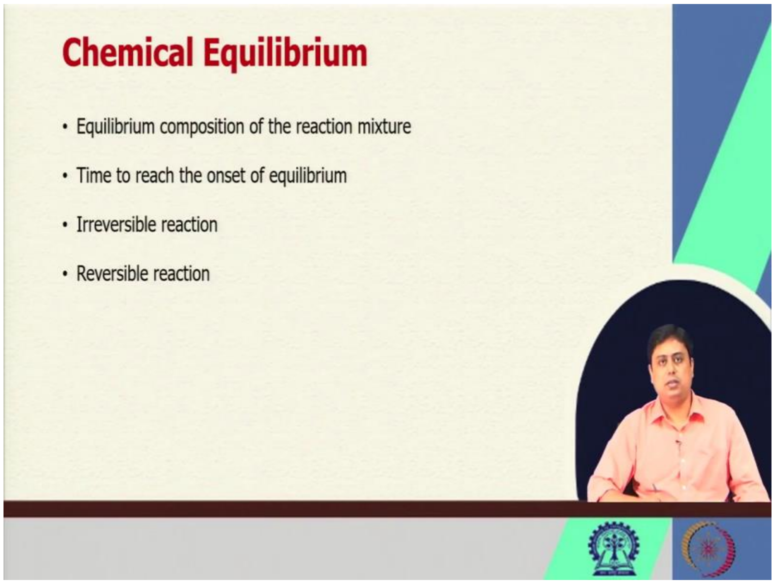
Material and Energy Balance Computations
Prof. ARNAB ATTA
Department of Chemical Engineering
Indian Institute of Technology, Kharagpur

Lecture –20
Introduction (Contd.,)

Hello everyone, welcome back in the NPTEL online certification course on Material and Energy Balance Computations. We were discussing chemical reaction stoichiometry its fundamentals and in the last class we have seen the concept of extent of reaction and how to calculate the product composition based on the concept of stoichiometry, stoichiometry ratio and extent of reaction.

(Refer Slide Time: 00:53)



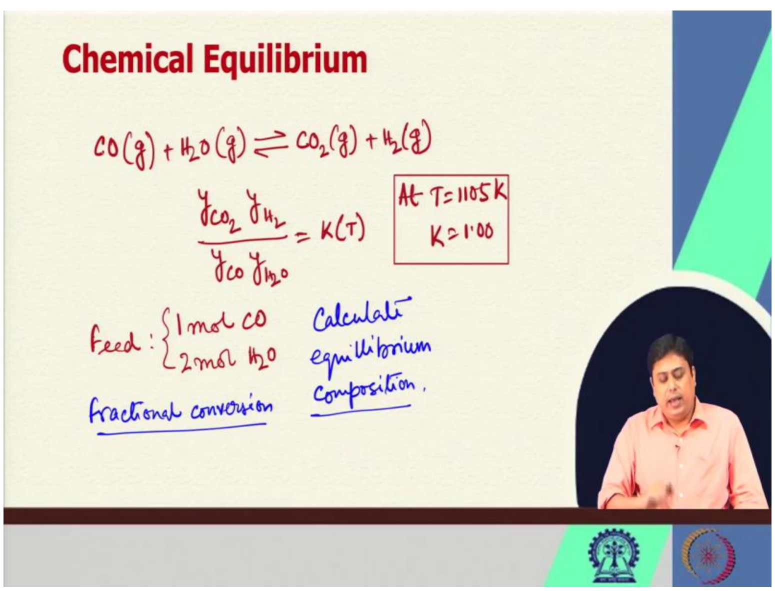
Now we have different types of reactions that we encounter in a chemical reactor. Now few reactions are irreversible. We say it irreversible that means the reaction goes in in only one direction that is the reactants are continuously consumed and generates product. But there are other reactions other sets of reactions where it happens that once some product is formed that product again dissociates or generates the reactants.

So, which means the reaction happens on both the way that is the reversible reaction. Now the point is that the questions that we often ask that what is the equilibrium composition for such cases of that reaction mixture and when we reach that equilibrium stage. The point is these are dealt in 2 different subjects will not go into the details of this equilibrium composition for the reaction mixture you would find in thermodynamics equilibrium thermodynamics.

And this onset of equilibrium or the time that is required that is dealt in chemical kinetics. But the point here we will understand that if such reactions are encountered while doing a material balance in a reactor how do we handle such scenario. So, the case the example of the reversible reaction that I mentioned is that say we have C_2H_4 and water. We start a reaction with this mixture and then what happens after a certain time this ethylene and water generates C_2H_5OH that is the ethanol and after a certain time we will see that this ethanol again generating C_2H_4 and H_2.

So, this is the reversible reaction that we identify when that happens and if we write it correctly so for such reaction what we will do? Whether our concept of extent of reaction can be applied to such scenarios or not. So, in such cases what happens once the concentration of the reactants decreases the rate of reaction decreases the concentration of product increases the rate of this reaction rate reversible or the reverse reaction rate increases and it finally reaches a equilibrium stage but the compositions further do not change.

(Refer Slide Time: 04:15)

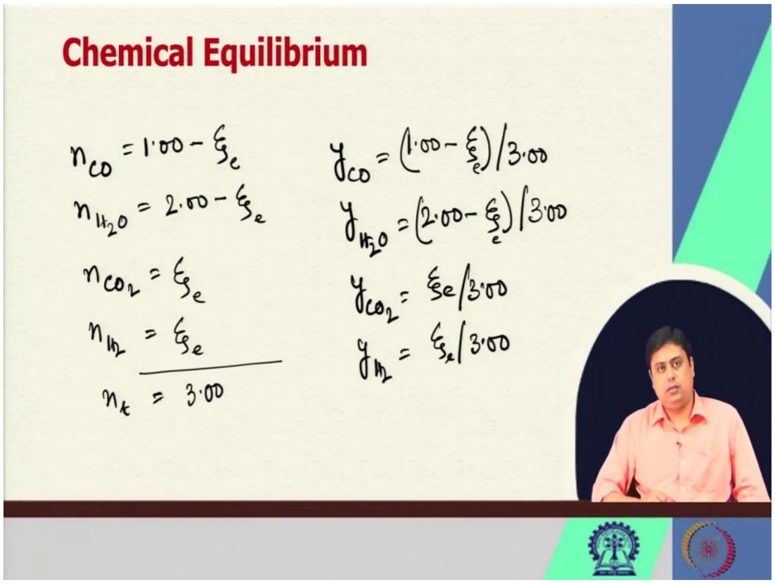


So, say we try to apply our same concept that we had for extent of reaction that we have seen in one case that is the chemical equilibrium of this reaction. So, this this is this is a quite famous reaction that happens. What this happens in case of several chemical process and we typically say this as the as the water - gas shift reaction. So, here we have carbon monoxide in gaseous form, H_2O in gaseous form generates CO_2 and hydrogen.

Now say the reaction is happening and it reached an equilibrium which is at 1105 K and at that point the molar fractions or the mole composition of the reactant and the product has this relation that is given here, where K is the equilibrium constant. This equilibrium constant has a value say 1 at this temperature this is of known information. The other thing that is known say the feed contains one mole of carbon monoxide and 2 moles of H_2O.

There is no carbon dioxide and hydrogen is in the feed. So we have to calculate here the task is we have to calculate the equilibrium composition and the fractional conversion of the limiting reactant. So, fractional conversion of the limiting reactant and what would be our equilibrium composition these are the things that we have to estimate for this problem. Now see whether we can apply our extent of reaction concept to this case or not and how we apply?

(Refer Slide Time: 07:30)



We certainly can apply the concept here as well to find out what is the product composition, here the product is at equilibrium. So, again from the stoichiometry we can see that this is in balanced form again stoichiometry means it must be valid which we can clearly see that the O we have 2 on the right hand side we have 2 the atomic carbon here is 1 and 1 and H_2 we have 2H's and 2H here. So, it is balance that means 1 mole of carbon monoxide consumes one mole of water H_2O to generate 1 mole of carbon dioxide and 1 mole of hydrogen.

And the other thing also is true that one mole of CO_2 consumes one mole of hydrogen to produce one mole of carbon dioxide and one mole of H_2O. So, now since in the feed there was no CO_2 and H_2O it is only one mole of CO and 2 moles of H_2O we consider that those are the reactants CO and H_2O and these are the products reactants and these are the products the extent of reaction here ξ and e stands for at equilibrium that the molar composition at equilibrium, the extent of reaction till the equilibrium.

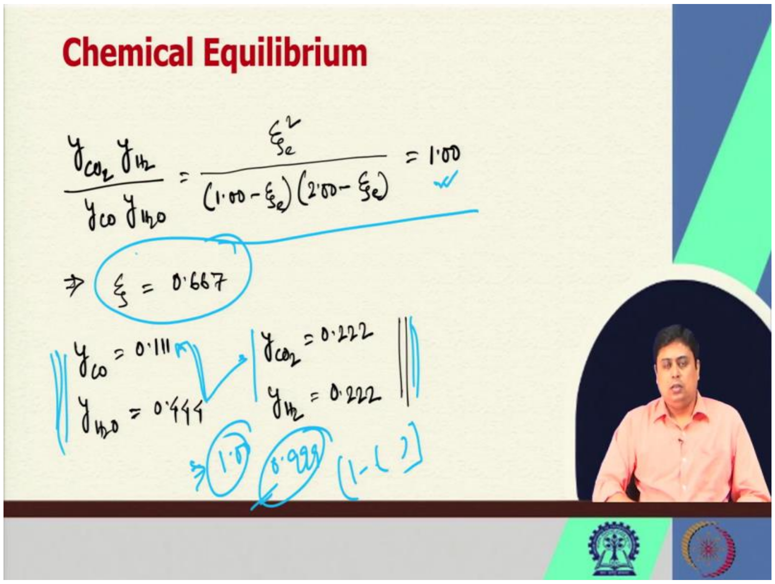
So, quite naturally we can write that at equilibrium number of moles of CO would be inlet + the nu × $(\xi)_e$, here the nu is 1 and it is reactant. So, it is – 1 and that is why it is 1 – $(\xi)_e$, e stands for the equilibrium this is the inlet feed composition or the inlet moles that has been given already. Similarly for water we see 2 moles this is also reactant. So it is also having 2 – $(\xi)_e$, 1 mole each of carbon dioxide and hydrogen is being produced. So, we have $(\xi)_e$ as the number of moles at equilibrium for both carbon dioxide and hydrogen.

So, which means the total number of moles at equilibrium considering we have one mole of CO and 2 moles of H_2O, what we have is three moles. So, that means the mole fractions of each component would be the individual value / this total value. Now in this problem what I did not explicitly mentioned is the limiting reactant its quite apparent that we have one mole of CO requires one mole of H_2O for this reaction to happen whereas 2 moles of H_2O is supplied.

So, which means the limiting reactant is of course the CO carbon monoxide. Now once we have the total number of moles we can calculate what is the molar fraction of the product? Now remember at that equilibrium. So, this is the equilibrium stage composition. Now here it is mentioned that the compositions are related by this relation such expressions are typically given. So, here now we can replace this y values to find out what is my extent of reaction.

So, the whole idea that we are going forward is to have a single variable calculation we are trying to generalize the formation so, that we can find out one single variable. So, that we can find out the composition of the output stream or the product stream.

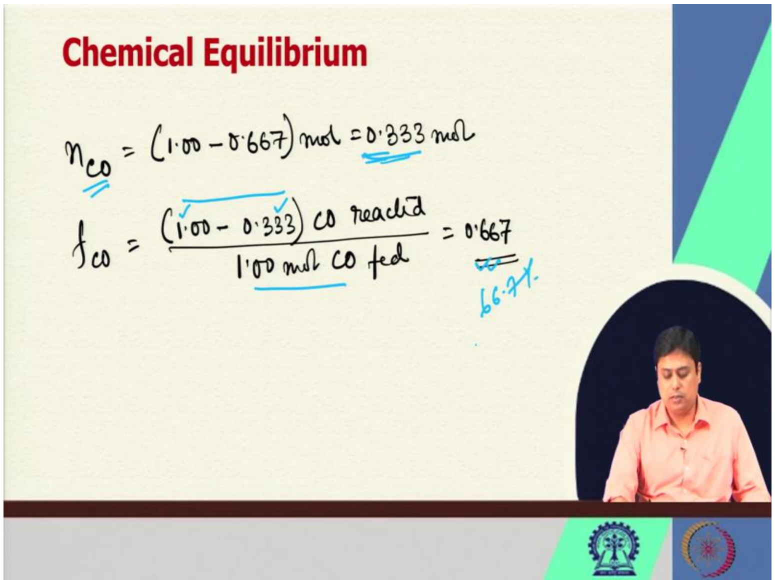
(Refer Slide Time: 13:09)



So, once we replace those values here in this expression this equilibrium constant value is known for that temperature we can solve these quadratic equations to find out that extent of reaction is this value. So, accordingly we find out what are my composition? Because these are the relation for each and every composition that we have seen. So, here one would just wonder or in order to cross check this value what you should do you should add all these totals and it should come out a value nearer to this one.

Because these are the mole fractions and indeed if you add these 4 values it is 0.999 or at the end one can also in order to ensure that what they can do is that they add all the any of the 3 and then subtract that from 1 in order to find the remaining composition or remaining constituents. So, we see that the extent of reactions and this is really beneficial when we have such equilibrium conversions or equilibrium stages and to find out their composition.

(Refer Slide Time: 14:58)

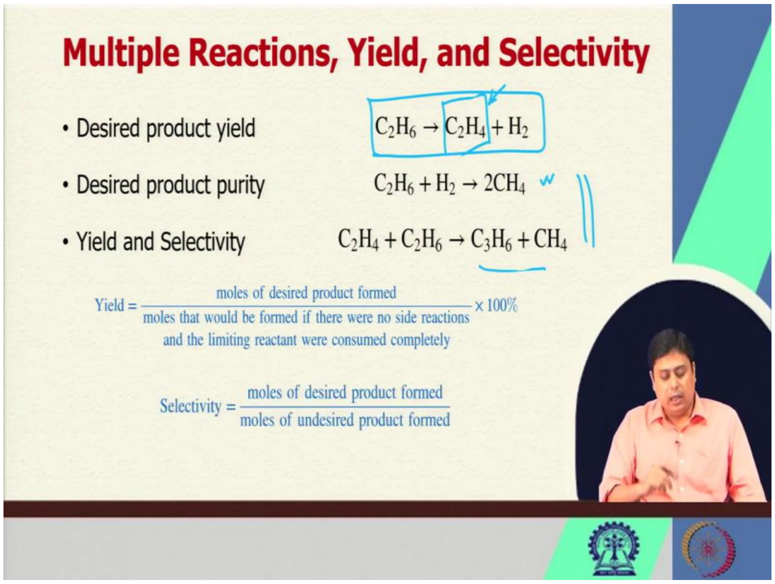


So, the remaining part was what is the fractional conversion of the limiting reactant. Now we have identified the limiting reactant is CO we see that the mole fraction of CO in the equilibrium stage or at the equilibrium stage when the product stream is 0.111 and we see that the extent of reaction here is 0.667. So, the number of moles of CO in the product is 1 – this thing that we have written here by the understanding on which we developed the extent of reaction concept.

So, this is the number of mole of carbon monoxide and in the equilibrium stage which means the amount that is reacted is basically 1 – this amount. If this is in the product stream this is what it has been reacted because this is the feed. The amount in the feed – the amount that has reacted it is in the output stream is the amount that it has reacted and this is happening per one mole of CO in the feed which means the fractional conversion is 0.667 or the percentage conversion is 66.7%.

So, I hope this concept is also clear to you that how we applied the extent of reaction concept for chemical equilibrium.

(Refer Slide Time: 17:34)



Now we move on to few other keywords that are also important when we will deal with reactions and the reactive system material balance and those are multiple reactions yield selectivity. Because it happens that hardly any reaction generates the pure product say our goal is to produce C_2H_4. So, we start with C_2H_6. So, we start with ethane to produce ethylene. Now say once this happens that C_2H_4 + H_2 the moment H_2O is generated and C_2H_4 this H_2 further reacts with ethane in order to form methane and not only that this ethylene also reacts with ethane to form propylene and methane.

So, these are basically undesired reaction that happens while our desired product is C_2H_4 because you see in these three reactions our aim is to find or is to produce only C_2H_4. But the second reaction does not produce even our desired product but it happens the third one what happens our desired product is further consumed in order to deplete whatever the formation has happened. So, the reactor engineers job is not only to optimize or enhance the production of this first reaction but also to minimize the chances of this side reactions that we called.

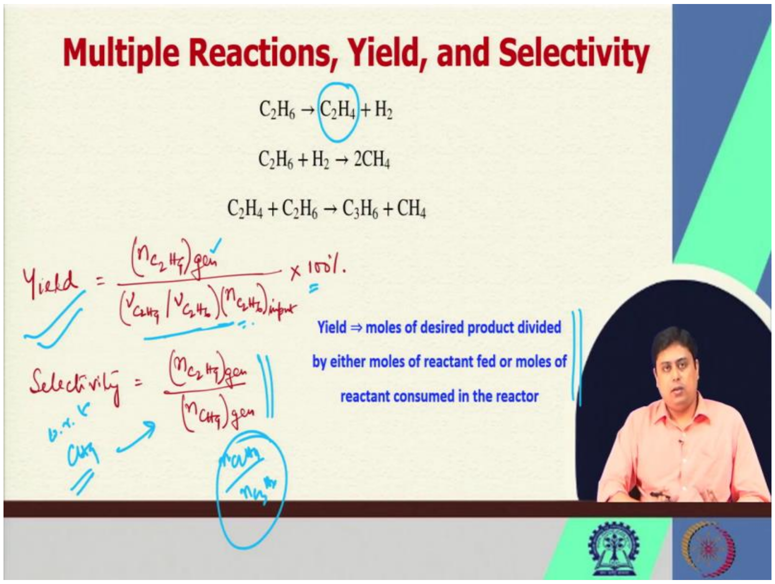
So, which means we have a couple of terms that we need to understand one is the desired product yield and its purity. So, yield and purity is what is important to us and in order to do that we define couple of parameters one is called the yield the other is called the selectivity. So, basically yield is the moles of desired product that we are trying to form and this is with respect to the moles that would be formed if there were no side reactions and limiting reactant were completely consumed.

This is called the yield the percentage of yield is multiplied by 100%. So, yield what happens the amount you are producing the fraction that you are producing of the desired product with respect to what could have been formed if there is no side reaction that means kind of a ideal scenario. So, you can think of the scenario or the situation as like this what you are actually producing and what could have been formed if there were an ideal scenario.

That is the yield of the desired product because these terminologies would be frequent when will solve the real problems of reactive system the other term related to this purity is the selectivity is the moles of desired product forming per moles of undesired product formed that is the selectivity with respect to a undesired product. Because here in the set of reactions you can see our desired product is ethylene undesired products are methane, propylene also hydrogen.

So, selectivity when we say selectivity we have to be specific that which one or which undesired product you are referring to or the problem statement is referring to that would be clearly mentioned. That the selectivity of the desired product with respect to hydrogen or with respect to propane or with respect to methane that fraction or the value would be given and then you can understand that this is nothing but the moles of desired product that we want per mole of that undesired product.

(Refer Slide Time: 23:31)



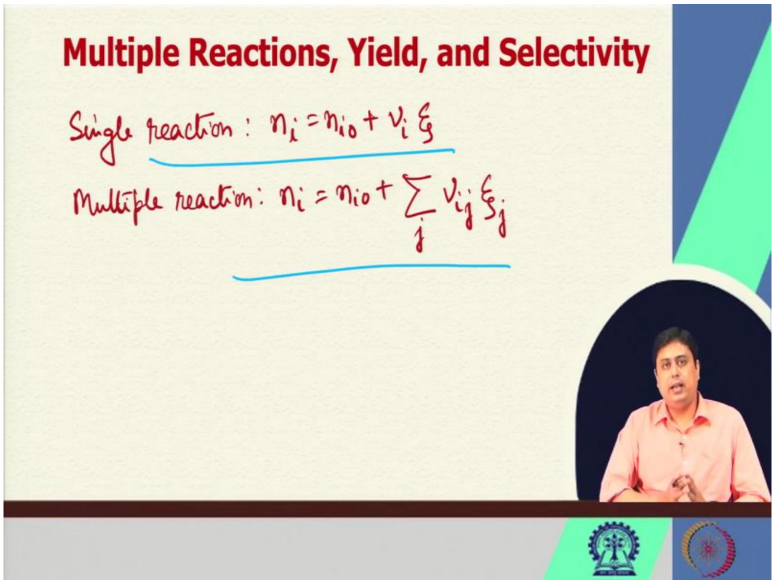
So, say again for this reaction that means what would be the yield? the yield would be remember this is our desired product. So, the moles of C_2H_4 generated per moles of the reactant that would be consumed in an ideal scenario which is here that we had to provide the C_2H_6 with the stoichiometry proportion which is the reactant multiplied by 100% this implies that here since it is only one reactant is there.

This is the only limiting reactant when there are multiple reactants or the species are there we had to identify which one is the limiting reactant for which we have to write in such a way such that the limiting reactant as if is consumed 100% that is the yield and in this case the selectivity is the C_2H_4 that is generated. Now as I mentioned selectivity with respect to CH4 then one can write this expression.

That the selectivity of ethylene with respect to methane is this one, if the value is given for selectivity with respect to propane that would be C_2H_4 / nC3H6. So, then there are also chances that the yield is slightly I mean defined in a slightly different manner. So, sometimes yield also means that the moles of desired product divided by either moles of reactant fed or moles of reactant consumed in the reactor.

So, if it is not mentioned explicitly like this that find the yield with respect to this reactant or the other reactant that is consumed in the reactor. We would typically go with the yield definition that is given here.

(Refer Slide Time: 26:43)



So what we have understood today the couple of concept that are important that is the extent of reaction, its application in chemical equilibrium, multiple reaction why selectivity and yield is necessary to define or to know. And finally here we will see whether the extent of reaction can also be applied to multiple reactions or not and if so, how we define that. So, similar to the single reaction when we have seen the extent of reaction like this.

For multiple reactions, we can also define or we can also find out the output stream composition or the product composition by the concept of extent of reaction. So we will pick it up from here in the next class because it requires the illustration of one example to combine with this concept. We will take it up in the next week, till then thank you for your attention.