Mass, Momentum and Energy Balances in Engineering Analysis
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Lecture - 12
Systems with Chemical Reactions

Welcome. So, far we have been dealing with systems which do not had any kind of generational consumption and generally the generations and consumptions are due to some kind of chemical reaction within the system. Now, as I told you in my previous lecture that the equations we are learning for the material balance or energy balance or momentum balance are applicable to non-reacting as well as to reacting systems.

So, now what I would do that I would take up some systems with the reaction terms in them ok. So, in this particular lecture what we shall do? We shall develop some basic understanding of how to consider the reactions chemical reactions in a given system before we move on to see the energy balance and mass balance where their chemical reactions are involved.

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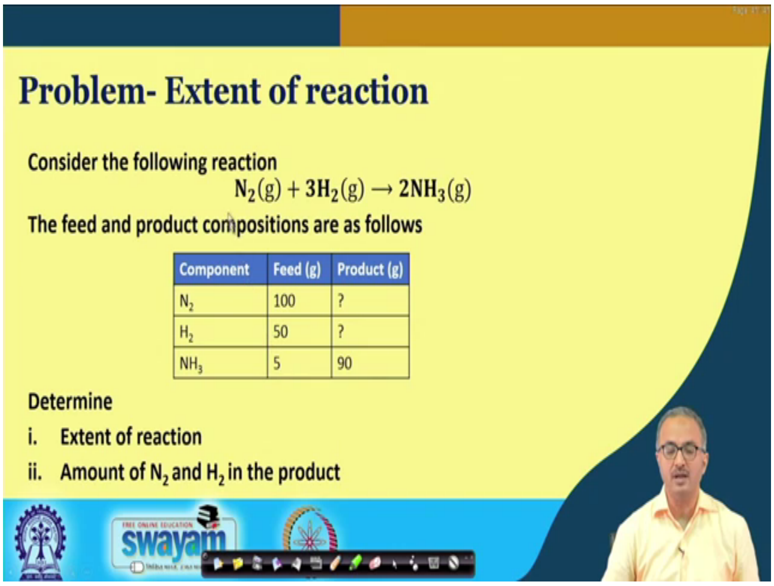

So, in this first we take to find out the extent of reaction that is to what extent a reaction would proceed. So, we shall be considering some very simple examples which you are perhaps aware of from your basic chemistry knowledge. So, here is first reaction I am showing which is showing that the nitrogen and hydrogen in both in gaseous state are reacting to form ammonia, also in gaseous state, and here we are not concerned with the operating conditions that is temperature, pressure or the catalyst being used, we are just concerned about the main reaction.

So, here we are given the feed and the product compositions as here that in the feed we have 100 grams of nitrogen, 50 grams of hydrogen and 5 grams of ammonia; that is the ammonia that is the product is also present in the feed, some amount of feed. Now, it could be due to various reason it could be that in an actual plant there could be some recycle streams or feedback streams, so which will contain some amount of the product ok. So, that may be coming in the feed. So, that is why it is not a surprising situation that we have some amount of the product in the feed stream also. And on the product side we do not know the amount of nitrogen and hydrogen, but we know the amount of the ammonia of 90 grams.

So, what we have been asked to do is to find out the extent of reaction and the amount of nitrogen and an hydrogen in the product ok. So, we have to fill up these two blank spaces.

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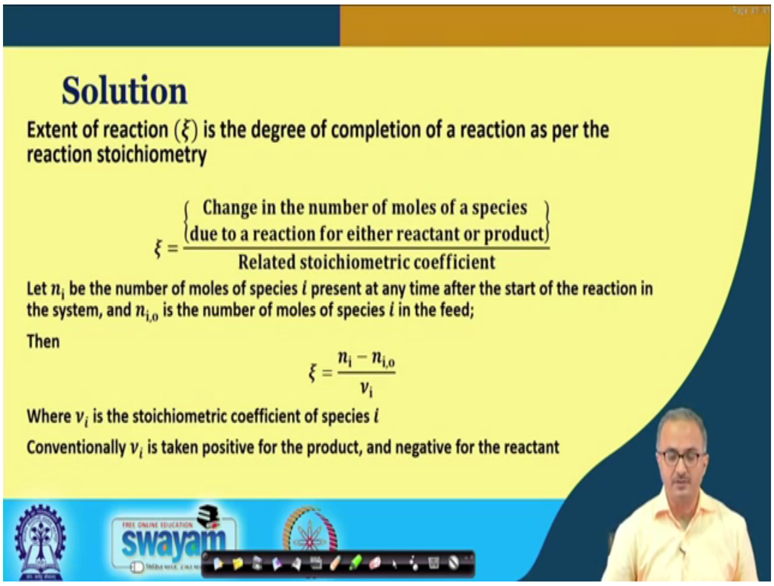

So, first what we do we understand what we mean by the extent of reaction. So, extent of reaction signifies the degree of completion of a reaction as per the reaction stoichiometry. So, as you know stoichiometry gives us the relative amount of the various products and the reactants. So, as per the stoichiometric reaction what is the degree what is the extent to which a reaction proceeds.

So, to find it out this is the way we find it out we take a ratio of the change in the number of moles of a species due to a reaction for either reactant or product and the related stoichiometric coefficient. So, this particular thing says that we can consider the change in the moles of any of the reactants or products and the respective stoichiometric coefficient. So, in this particular example we can see the nitrogen has a stoichiometric coefficient of unity, for hydrogen it is 3, for ammonia it is 2 ok. So, we have to put the respective stoichiometric coefficient over here. And the extent of reaction which we get by considering any of the reactant and the products will come out to be the same.

Now, in terms of symbols let us see that if we take n i to the number of moles of species i present at any time after the reaction has started, and n i naught is taken as the number of the moles of species i in the feed ok. So, the extent of reactions taken as the amount which is present minus the amount which was there initially divided by the related stoichiometric coefficient. Now, this stoichiometric coefficient is taken to be positive for a product and negative for a reactant conventionally. So, with this particular definition of the extent of reaction we are now prepared to solve the problem.

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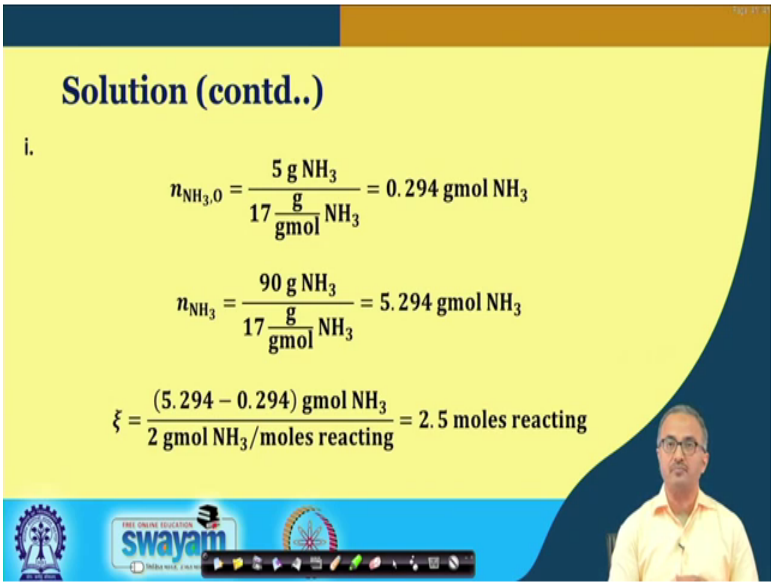

So, here we have the statements that the amount of ammonia present is this particular thing that 5 grams ammonia divided by 17 which is 0.294 gram mole of ammonia. Then, we take the ammonia present in the product to be 90 gram, again by 17 gram per gram mole is the molecular weight of ammonia we take this the gram mole of ammonia present finally. So, in terms of ammonia because we do not have the composition of nitrogen or hydrogen in the product. So, we have to find out the extent of reaction in terms of ammonia. So, we find out that this is the final amount, this is the initial amount and divided by 2 gram mole of ammonia per moles reacting ok. So, this is the thing we are getting 2.5 moles reacting.

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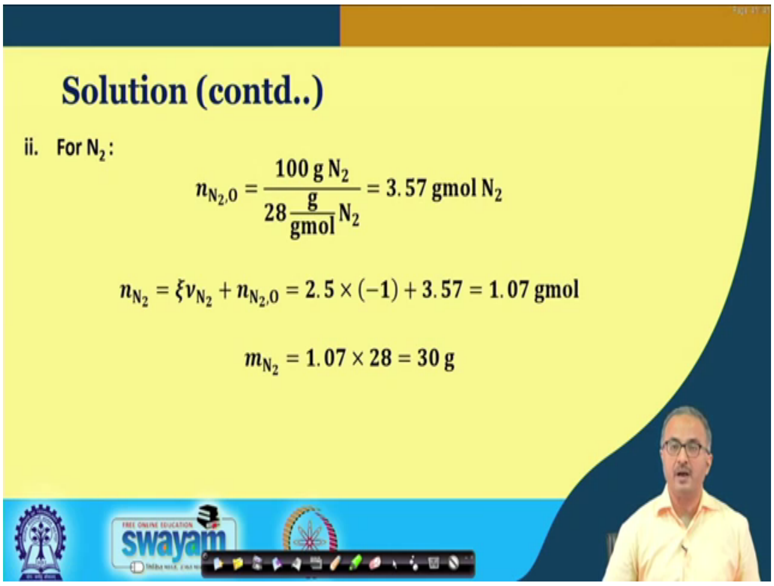

Now, once we get the value of the extent of reaction we can now find out the final amount of nitrogen. So, for that first we find out the initial amount of nitrogen that is 100 grams of nitrogen divided by its molecular weight that is 3.57 gram mole of nitrogen. And now, from the definition of the extent of reaction we find out the final amount of nitrogen as the stoichiometric coefficient into the extent of reaction plus the initial amount of nitrogen and we put the respective values over here and we get the final amount of nitrogen is 1.07 gram mole. And in terms of the mass we simply multiply this with the molecular weight of nitrogen, so this many grams of nitrogen are present in the product.

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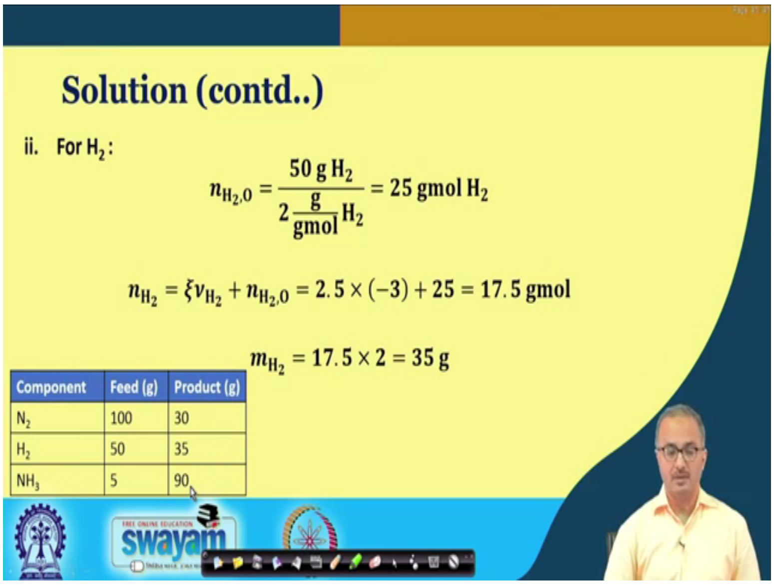

Similarly, we move on to the hydrogen. So, we find out the gram moles of hydrogen by dividing the mass of hydrogen present in the feed by the molecular weight of hydrogen this is 25 gram mole of hydrogen. Again, using the definition of the extent of reaction we find out the final amount of the hydrogen by plugging in the extent of reaction the stoichiometric coefficient of hydrogen which is the negative sign and this is the initial amount of hydrogen. So, we get this is the value and this is the mass of the hydrogen present in the feed. So, we get that in the in the sorry in the product. So, we get that the 30 grams of nitrogen 35 grams of hydrogen and 90 grams of the ammonia in the product.

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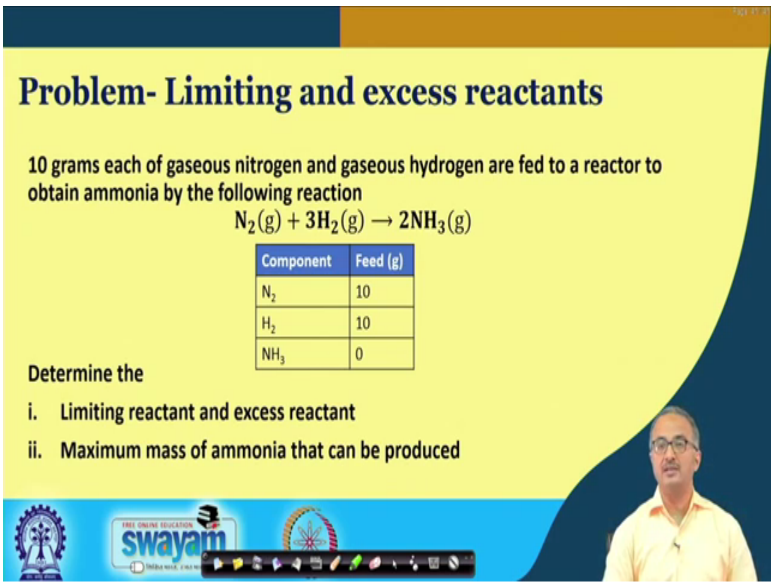

Next, we move on to another system in a chemical reactions we are also interested to know that when there are many reactants present then it may so happen that some reactants get exhausted before the reaction goes to completion. So, any reactant which gets exhausted for the first time by only the reactions not by any kind of leakage or anything that particular reactant is called the limiting reactant and it decides the extent to which a reaction would proceed ok.

So, here in this particular problem we have to find out the limiting reactant and any other reactants other than the limiting reactants will be the excess reactant. So, here we have the 10 grams each of gaseous nitrogen and gaseous hydrogen are fed to a reactor to obtain ammonia by the following reaction. So, this is the same reaction as before and this is the amount of the feed 10 grams of nitrogen, 10 grams of hydrogen and there is no ammonia in the feed. We have to determine the limiting reactant, the excess reactant and the maximum mass of ammonia that can be produced ok.

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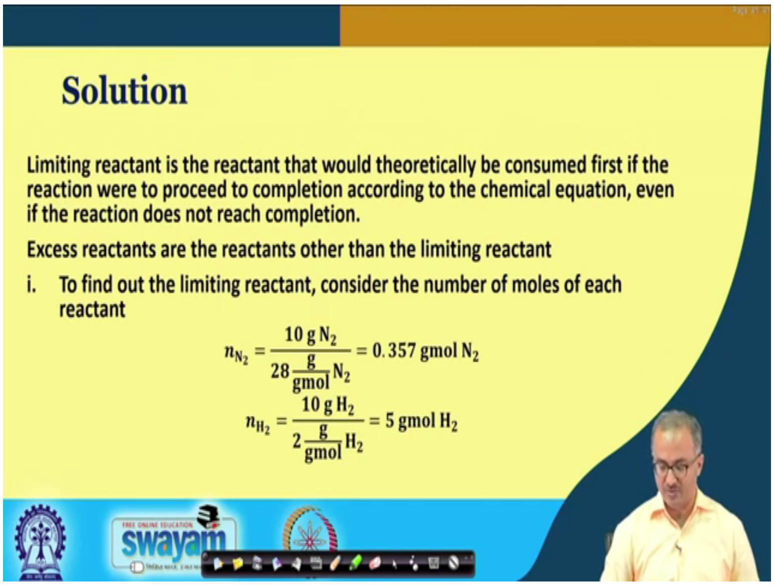

So, you one thing you must understand that the amount given in terms of the mass is same, but that does not mean the limiting reactants are both because the reactions proceed in terms of the moles ok. So, put we have to put in terms of moles.

So, first let us see the definition the limiting reactant is the reactant that would theoretically be consumed first if the reaction were to proceed to completion according to chemical equation even if the reaction does not reach completion. It means that as soon as the particular reactant gets exhausted the reaction will automatically stop ok. And the excess reactants are the reactants other than the limiting reactant.

So, first to find out this limiting reactant as I mentioned that these everything all the masses have to be first converted to moles. So, we find the number of moles present in the feed as 10 gram by the 28 gram per gram mole, the molecular weight of nitrogen and these many gram moles of nitrogen present and similarly we find out the number of moles of the hydrogen. So, in the molar terms we find that nitrogen is less than hydrogen.

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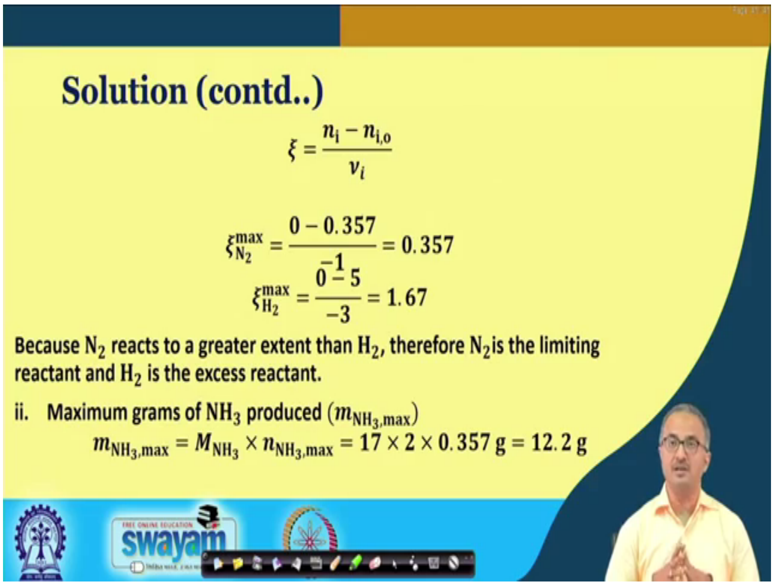

Now, we find out the extent of reaction for both the cases. So, with respect to nitrogen if you find that this is the; this is the value we find for the nitrogen that is the maximum extent of reaction and this is the maximum extent of reaction in terms of hydrogen; that means, if all the hydrogen and all the nitrogen gets exhausted ok. So, here we find that if nitrogen get exhausted then this is the extent of reaction. If hydrogen get exhausted this is the extent because it is getting exhausted. So, we are putting the final amount to be 0 in both the cases ok.

Now, this does not contradict my earlier statement that the extent of reaction is invariable with respect to any reactant and product because we are looking at the whole thing at a given time, but here they are different because we are looking at the maximum extent, So, here we find because the nitrogen reacts to a greater extent ok. So, nitrogen becomes the limiting reactants and hydrogen is the excess reactant, so that means, what that even if equality of mass does not mean that both the reactants are limiting or excess. So, we have to first putting in terms of the moles.

Now, once we know that nitrogen is the limiting reactant, we can find out the maximum amount of ammonia produced because the maximum amount will be decided by the amount of nitrogen and not by the amount of hydrogen. So, what we see here in the reaction that, one mole of nitrogen gives rise to two moles of ammonia that is the stoichiometry is saying. So, if we have 0.357 moles of nitrogen getting exhausted fully that will lead to 0.357 into 2 this many moles of ammonia and when we multiply that many moles with the molecular weight of ammonia, we get the mass of ammonia produced due to exhaustion of all the nitrogen or the limiting reactant.

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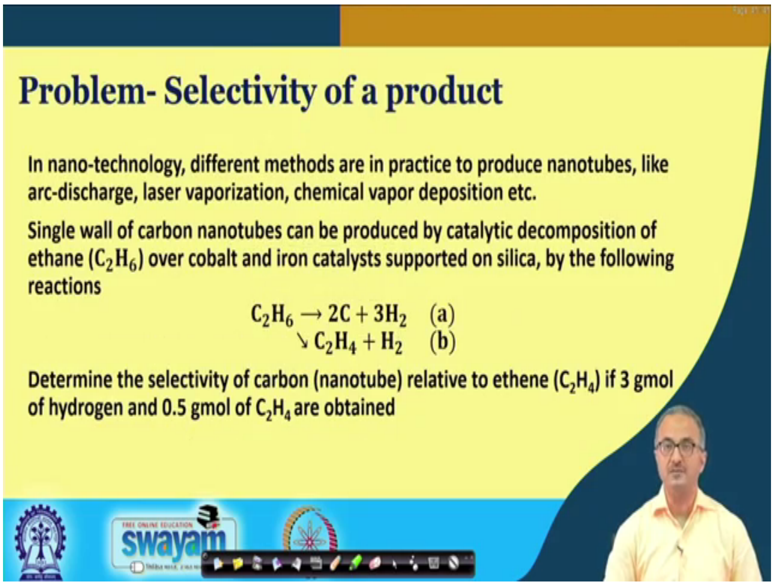

Next, we come to another problem in this problem we shall be learning about the selectivity. So, here we take a again practical problem in nanotechnology we produce the carbon nanotubes by various processes like arc discharge laser vaporization chemical vapor deposition etcetera.

Now, single wall carbon nanotubes can be produced by catalytic decomposition of ethane that is C 2 H 6 over a catalyst that is cobalt and iron catalysts supported on a silica matrix and this is the reactions. So, here we see the main reaction is this we are decomposing it, so there is only one reactant ok. So, this C 2 H 6 is decomposed to give carbon and hydrogen. But this is not the only reaction that takes place in the system there is another reaction also goes on that is also decomposition, but in this case this is a partial decomposition of ethane and in this case we get ethene and hydrogen and you know that ethane is an alkane and ethene is an alkene ok.

Now, because we are getting two types of products in this carbon is the desired product and anything other than carbon is the by-product ok. So, C 2 H 4 is the by-product and so is hydrogen. We have to find out the selectivity of carbon nanotubes relative to ethene that is C 2 H 4 if 3 gram mole of hydrogen and 0.5 gram mole of ethane are obtained. So, we have been given the amount of ethene and the amount of the hydrogen, total amount of hydrogen which are coming from both reactions a and reaction and b.

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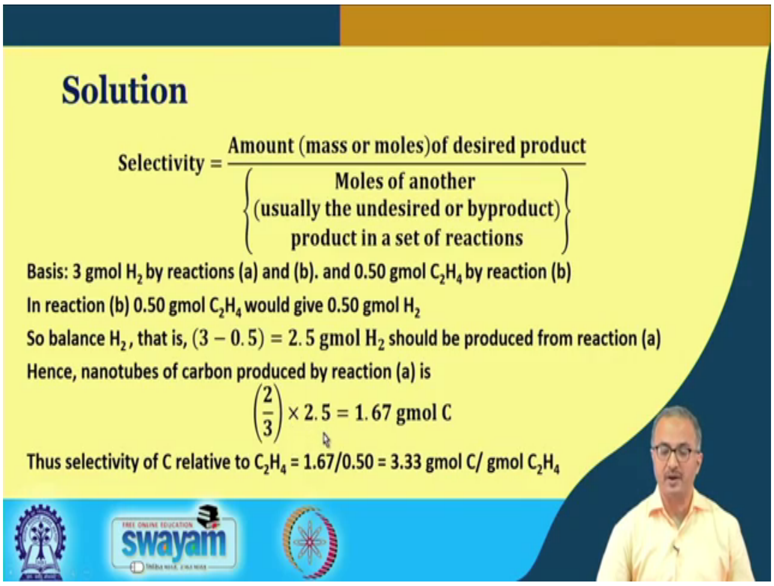

To solve this problem first let us understand the meaning of selectivity. Selectivity actually gives whenever when we have multiple reactions going on, so we shall be having some desired product and rest of the things will be undesired products or the by-products ok. So, we mean that how much of the desired product is formed with respect to the other undesired products. So, ideally, we should have as much selectivity as possible because we do not want to have the undesired or the by-products ok.

So, here we have the definition that amount of the ratio of the amount of the desired product this amount may be in terms of mass or moles divided by moles of another product ok. So, here we find that in our problem which has been given that basis is 3 gram mole of H 2 by both reactions a and b and 0.5 gram mole of ethene by reaction b.

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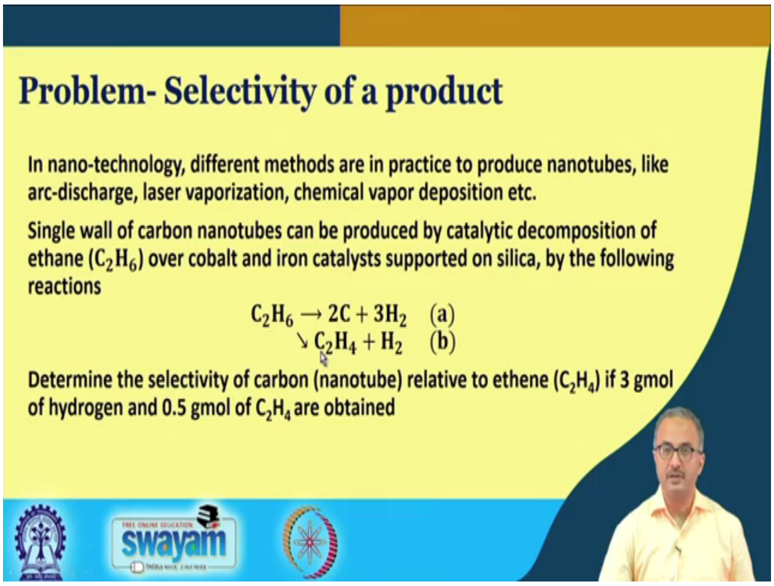

Now, from reaction b we find that the amount of ethene and the hydrogen in terms of moles is the same; that means, when we have 0.5 gram mole of ethene produced we shall also be having 0.5 gram mole of the hydrogen produced from reaction b. That means, what? That 3 minus 0.5 that is 2.5 gram mole of the hydrogen will be produced from reaction a.

Now, please note here that here it could be this is the amount of another product could be in terms of both mass and mole. Now, you see here that the nanotubes of carbon produced by reaction a is like this that two-third of 2.5 that is 1.67 gram mole. How you find this? This is again you can find out that this. If you go back to this reaction you can see that for 2 moles of carbon we are having 3 moles of hydrogen ok. So, with this knowledge we find that the amount of carbon produced will be because this is the amount of gram mole of hydrogen produced from reaction a. So, 2 by 3 into 2.5 that is 1.67 gram mole of carbon ok. And the carbon is produced only from reaction a and not from reaction b. So, selectivity is now very simple that we take the gram mole of carbon produced divided by the gram mole of the ethene produced and this is coming out to 3.33 gram mole of carbon per gram mole of ethene.

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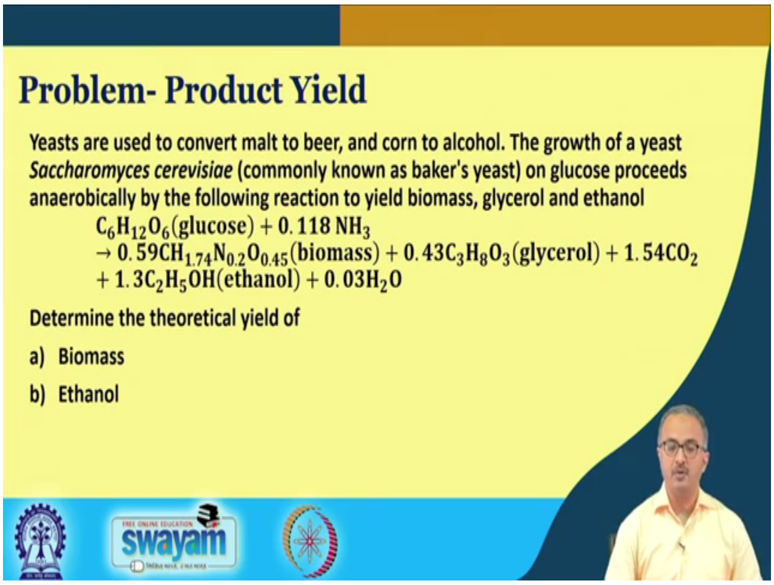

Next, we come to a problem where we are looking to the product yield ok. So, in this case we are taking a problem from the biotechnology. Here we are we know that we are using yeast, yeast we use also in our day to day life the yeast are used to convert malt to beer or corn to alcohol.

Now, there is a particular yeast that is saccharomyces cerevisiae which is called baker's yeast to convert this glucose anaerobically to yield some biomass glycerol and ethanol. So, this is the particular reaction over which this yeast acts and to give out the various types of products ok. Now, we find that with this reaction we have to find out the determine the theoretical yield of biomass and ethanol.

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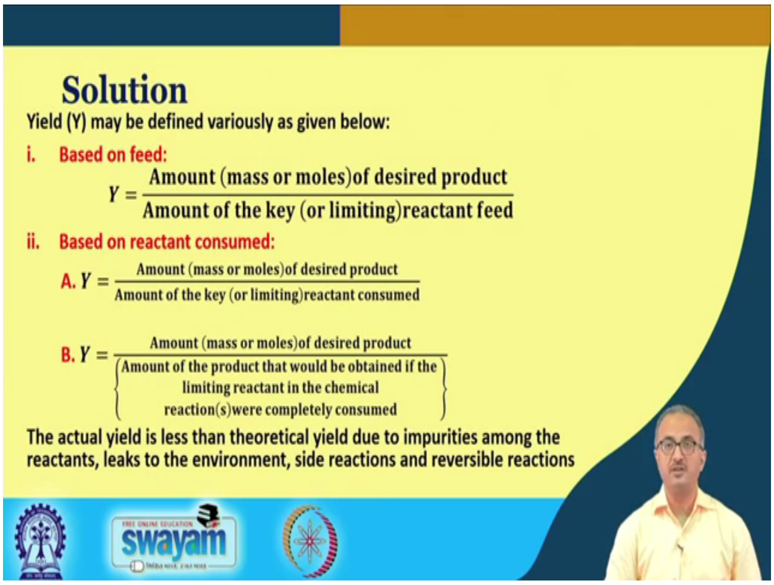

To solve this problem, we shall first look into the definitions of yield. Now, this yield may be defined in various manners so, first definition in terms of the feed. So, in this case the definitions is like this is the ratio of the amount of the desired product to the amount of the key or the limiting reactant fed.

Second definition is based on the reactant consumed. In this case first definition is like this the ratio of the amount of desired product divided to the amount of the key of the limiting reactant consumed. It is similar manner is the ratio of the amount of the desired product to the amount of the product that would be obtained if limiting reactant in the chemical reactions were completely consumed ok. So, the difference is this that in this case it is at any given point where it is not completely consumed and this is with respect to the time that is completely consumed ok.

Now, you see that the actual yield will be less than the theoretical yield, why because there could be impurities among the reactants, there could be leakages from to the environment, there could be other side reactions and other reversible reactions.

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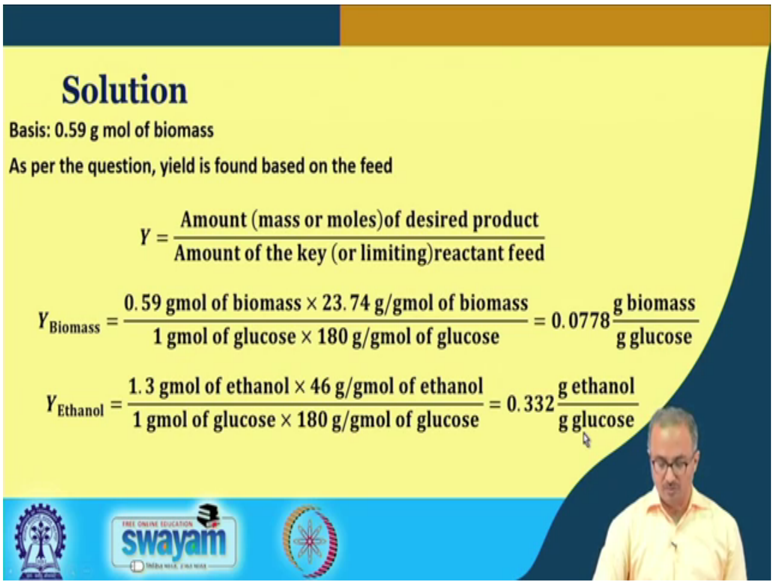

So, we have been asked to find out the theoretical yield for this we take the basis as 0.59 gram mole of biomass and as per the question we take the definition for the feed.

So, here we have this definition. So, first we find out from the particular reaction the amount of the biomass, so this many gram moles of biomass was produced and this is the given molecular weight of the biomass. So, we find out this is the gram of the biomass and for 1 mole of the gram mole of the glucose this is the glucose molecular weight and you can see this is the yield of in grams of biomass per gram of the glucose.

Next, for the ethanol again we see this many ethanol are there and this is the 46 grams is the gram per gram mole is the molecular weight of ethanol and this is same as the previous problem and we find this is the yield of the ethanol per amount of the glucose.

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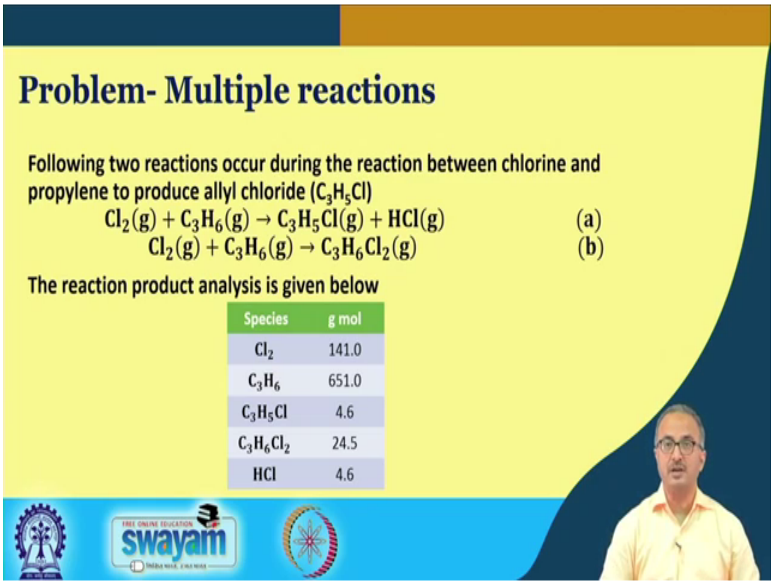

Next, we come to a situation where we are going to take help of all the definitions we have used so far for a system of multiple reactions. So, here we have the two reactions, these two reactions are occurring simultaneously and our desired product is the allyl alcohol, so this is the particular product of interest ok. But we are finding we have another product also formed along with this. So, we have been given the product analysis as this. So, we have all chlorine and other components in the product.

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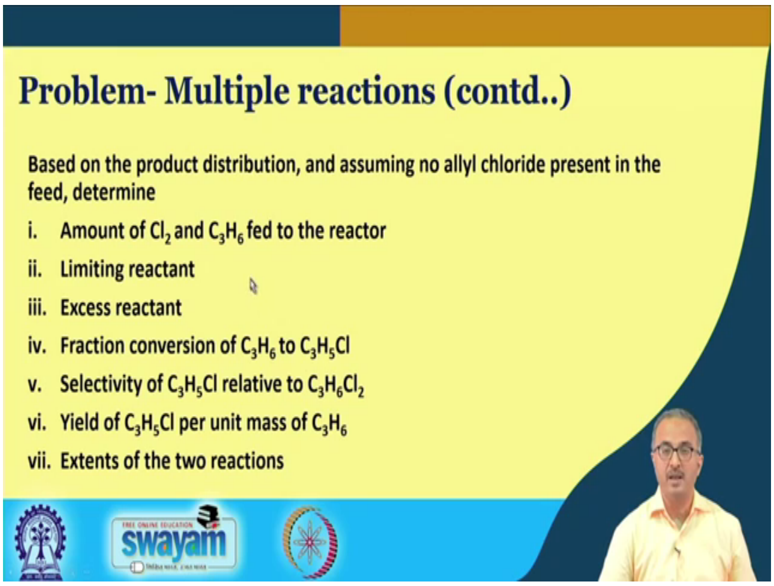

And we have been asked to find out the amount of chlorine and the propane that is fed sorry, propene fed to the reactor, the limiting reactant, excess reactant, fraction conversion of propene to allyl alcohol and selectivity of this, this, relative to this C 3 H 6 Cl 2 and yield of this allyl alcohol per unit mass of the propene and extents of the two reactions.

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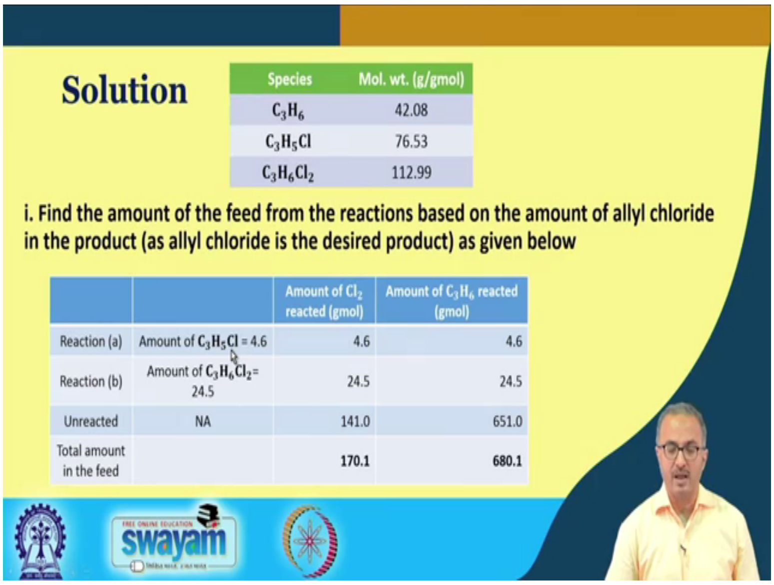

So, we write the molecular weights of the components of our interest and we also see the amount of the chlorine and the propene that are present in the feed. So, for even though these are not given in our problem, but we find it out in this particular fashion that let us consider first reaction a. Now, in this we find that this many gram moles of C 3 H 5 Cl are produced and for the same we find that the same in this particular thing 1 mole of this gives 1 mole of H Cl and consumes 1 mole of Cl 2; that means, the moles of Cl 2 will also be 4.6 and the moles of C 3 H 6 will also be 4.6.

Similarly, from stoichiometry for the second one we also find that 1 mole of this compound will be consuming 1 mole of Cl 2. So, we have same moles of Cl 2 and the same 1 mole of C 3 H 6. So, we have again same moles of C 3 H 6. That means, what? That this is the total amount that has got reacted. So, this is the 141 and this is the total amount that is got reacted here ok.

So, total amount in the feed will be this summation plus the amount which gets unreacted which we are getting from this product composition ok. So, we add it up these two components which are in the product with these two things which have got reacted. So, we get the total amount which was present initially in the feed ok. So, this answers our first part of the question.

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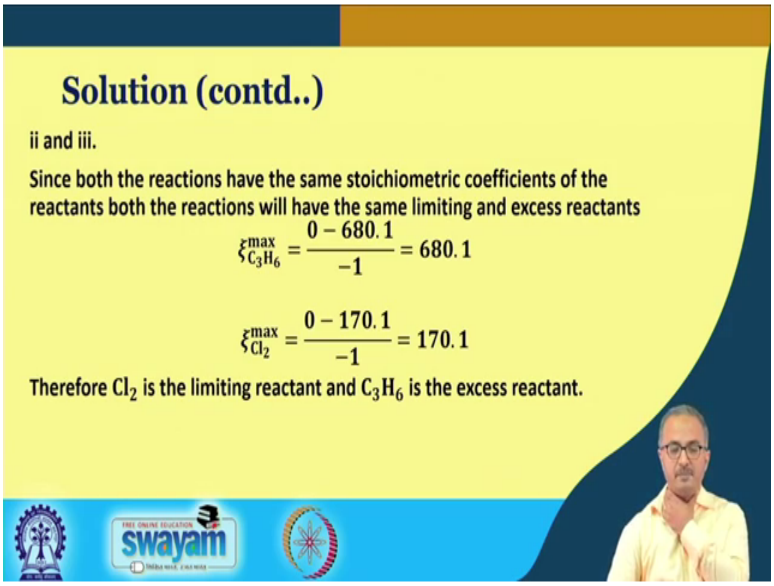

Second part and third part, relates to finding the limiting reactant and the excess reactant. Again as the previous problem what we do we find out the maximum extent with respect to the two reactants that is the propene and the chlorine. So, assuming their final amount to be 0 and these are the initial amounts of these and these are the stoichiometric coefficients with a negative sign because they are the reactants, we find out the extent of reaction with respect to the two components. And we find that because this value is less than this value, so chlorine is the limiting reactant and propene is the excess reactant.

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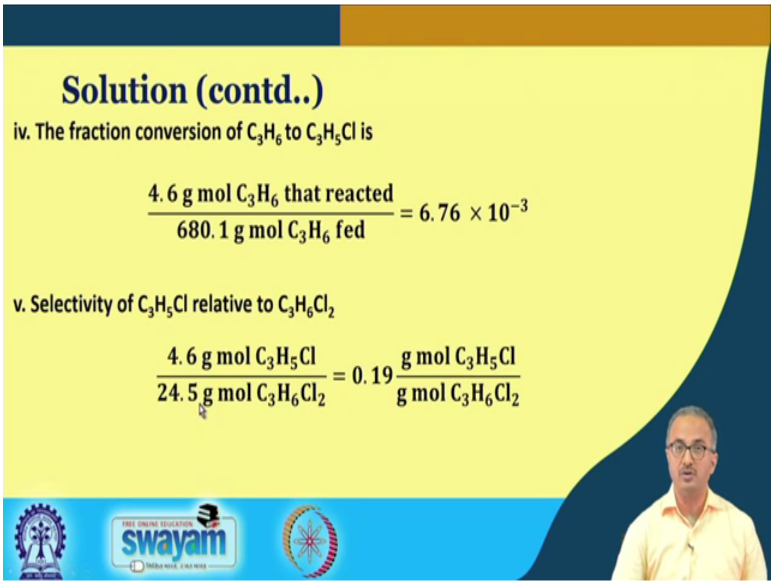

Now, for the fraction conversion of C 3 H 6 to this. What we simply do? From the given data which we have just generated that 4.6 gram of C 3 H 6 got reacted and this much amount of the C 3 H 6 was present in the feed. So, we get the fraction conversion like this for propene to C 3 H 5 Cl and then selectivity of C 3 H 5 Cl relative to C 3 H 6 Cl 2 for this again we go back to the product analysis and from there we find these many gram mole of C 3 H 5 Cl was formed for 24.5 gram mole of C 3 H 6 Cl 2. So, simply dividing these two we get the selectivity of allyl alcohol with respect to C 3 H 6 Cl 2, allyl chloride sorry.

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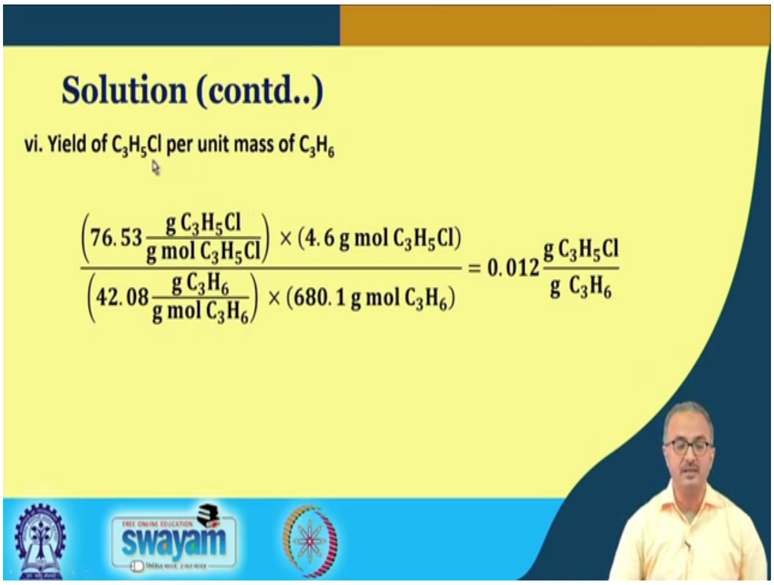

And here we have the yield of the allyl chloride per unit mass of propene, for this again we go back to the definition with respect to the feed. So, this is the amount of the sorry this is the amount of the allyl chloride formed and this is the molecular weight of allyl chloride, and this is the molecular wright of the C 3 H 6 and this is the amount of C 3 H 6 taken initially by dividing these two things and this masses we get the yield of C 3 H 5 Cl with respect to C 3 H 6.

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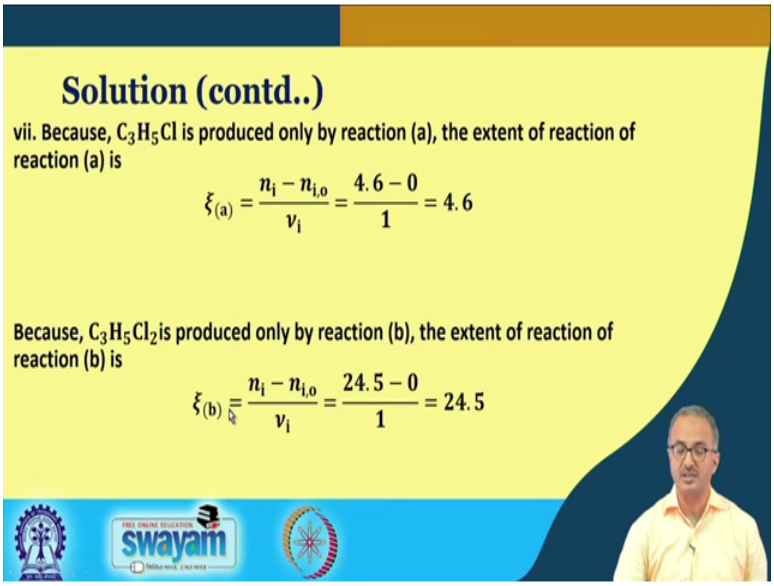

And lastly, we have to find out that the extent of the reaction we have to find out the now you see that here we have the C 3 H 5 C l is produced only by reaction a ok. So, what we find? The extent of reaction from this we find out that 4.6 was there finally, and there was no C 3 H 5 Cl initially in the feed and this is the stoichiometric coefficient of the C 3 H 5 Cl and with a positive sign because its the product. So, this is the extent of reaction.

Once we know the extent of reaction now this is the C 3 H 5 Cl 2 is produced only by reaction b. So, we have to find out the extent of reaction of this particular component separately. So, because these are from two different reactions, so we cannot take the extents of reaction from this equation to this equation. So, we have to find it out separately for the two reactions. So, for the reaction b we are doing it with respect to C 3 H 5 Cl 2 and we find out this is the amount that is present in the product this is the amount which is present in the feed that is that is nothing of this was present in the feed. So, doing this subtraction and again putting the stoichiometric value with a positive sign we get the extent of reaction for this second reaction.

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And these are the two books you can refer to know more about these. And further what we shall do that we shall see that with this, particular fundamentals on the chemical reactions, we shall try to look into those systems where we have the chemical reactions and do some mass balance and energy balance problems.

Thank you.