Engineering Thermodynamics
Dr. Jayant Kumar Singh
Department of Chemical Engineering
Indian Institute of Technology Kanpur

Week-12
Lecture-54
Chemical Reaction

Welcome to the Chemical Reaction part 2 lecture. In this lecture we will discuss about percentage theoretical air and some applications to understand it. Let's talk about combustion process in combustion process, normally we would have discussed that some temperature is required minimum only then your combustion will happen i.e. it will burn But there should be many reasons to burn to burn completely that the entire fuel comes in CO2, H2O and not in any other form of carbon completely combust, completely burn, completely burn. So, in such a case, there are many assumptions when the combustion is complete. First, the mixing should be done very well. And your temperature range should also be good. So, all these things, the practical constraints because of that, many times what happens is that the minimum air that is needed to burn, we use that more. So, sometimes excess air will come out. Like we have taken the fuel and put air. So, the air will be more than sufficient. Because of this, your CO2 H2O came out. Because this was CnHm, in the final product, CO2 H2O will be there. And excess O2 will also be there. Of course, the inner top nitrogen will also be there. Excess O2 because we have considered more air. So, in the normal process, we take excess air. Because combustion is not normally complete and there are many reasons for that. So, if it is complete in the ideal case, then the carbon in the fuel will be converted into CO2 and the hydrogen will be converted into H2. And if there is a sulfur in the fuel, then it will be converted into SO2. In complete combustion, you have more unburned components like CO, H2, CO etc. And especially, you need to understand that oxygen has a tendency to burn with hydrogen. So, it will make water quickly. But carbon makes it difficult. Carbon is not converted easily. And there are many reasons for this. First, you don't have sufficient oxygen. then it is possible that your complete composition is not happening. Second, mixing is very important in the composition chamber. And it has to be given time. Time means, you assume that you put it immediately and your composition started, and the product was made. It takes time in this reaction. So sometimes you have to make contact and eventually there will be a transient period and then a steady period where your product does not change in composition. So insufficient mixing is also a reason for the process of in-completion. Second, if the temperature is high, then there will be a dissociation. If there is a dissociation, then you can get different compounds. As you have seen, these can come in a higher temperature. This is an ideal scenario where you have to convert C into CO2, H into H2O, C into carbon dioxide and hydrogen into water. If we take this amount of minimum air which completely combusts the fuel, then we call it theoretical air. 100% theoretical air. So minimum amount of air needed for the complete combustion of a fuel. This is called chemically correct amount of air and 100% theoretical air.

For example, methane. We took 2 moles of oxygen and we had to take additional because it is air. So, the air is done. So, if we take this amount, then this C is CO2, H4 will be in water and the rest of the nitrogen will be released. So, what is this? This is chemically correct amount of This is a stoichiometric relation and this amount is 100% theoretical. and this is your theoretical combustion means this is your theoretical You will not get free oxygen in this product. With no free oxygen in the product.

In the complete combustion process, there is no free oxygen. We put as much amount as required. And this is your theoretical combustion. Now what happens is that this is not a reality. Because you play kinetics, you need time, you need mixing. And the effect of temperature and pressure also affects. excess air is added to the stoichiometric amount. This is more than theoretical air. So, the definition of excess air is the amount of air in excess to the stoichiometric amount. The amount you need more than theoretical is called excess air. And how do we express this? We express this in percentage excess air or percentage of theoretical air. If we say that 50% excess air is added, 100% is theoretical, 50% is access. So how much is the total amount? 150% is theoretical. If 200% is access, 100% plus 200% is theoretical. That is 3 times. That is 300% is theoretical. 90% is theoretical. That means it is 10% deficient. Deficiency of air means the amount of air which is less than theoretical amount. We also express this as percentage deficiency of air. So, this is the basic definition. It is important to understand that this definition will be used in your question. Another term is equivalence ratio. Equivalence ratio is the ratio of actual fuel. So, AF actual. ratio of the actual fuel ratio to the stoichiometric fuel ratio. The actual divided by theoretical. Either we can call it theoretical or stoichiometric. So, this is your equivalence ratio.

Now let's talk about the gas analyzer. How do we analyze the product? How is the composition of the product? If your composition is complete, then it is very easy. Then you have balanced the elements. And as we explained in the previous lecture, W and all the moles of the product. You have defined it as WZ Then you can define the elemental balance, carbon, hydrogen, oxygen, nitrogen You can take out the terms and amount of moles Then you can take out the composition according to the mole fractions But the problem is that if in the actual combustion process You may not have complete composition Then you cannot do analysis like this For this you have to measure the composition of the product. There is a device which normally does this. It is called Orsat gas analyzer. And it is commonly used to analyze the composition of the product or the gas. It normally reports on a dry basis. It means that there will be no water vapor in it. So, it will report on a dry basis how much is your analysis. And this You can read more about this later. But when we ask questions, we will assume that the composition is being taken out through this. Now we will do some examples which will help you understand the defined example better. This is a sample of a coal sample. This is the coal sample which is used in the chamber. The composition of this is CH2O2N2S Sulfur Ash. and we are using theoretical air in it. We are putting it in the combustion chamber and the product is coming out in the form of gases and ash. Now, they are saying that if you ignore the ash content, then you tell me what the mole fraction of the product in the composition form is and what is the apparent molar mass of the product of gases. and the air-fuel ratio is also required for this combustion. So, you have to calculate the theoretical air as well. so, there are two or three important things in this. First of all, you should know the molecular mass of all the molecules. So, like C, H2, O2, N2 Instead of N2, let's take air and sulfur. So, C is 12, this is 2, all of this will be in kg per kilomole unit. And O2 is 32, air is 29, sulfur is 32. So, all of this is in kg per kilomole. We will assume that the sample we are using is 100 kg of coal. This is the basis. We call this basis many times. We will do some analysis on the basis of this. First of all, we have to find out the moles of the coal. What is the number of NC? What is NC? NC NH 2, NO2, N2, and N of S. If we take out the values, it will be very easy to get the values. For example, we will use carbon. Carbon is 84.36 kg. We have taken 100 kg of coal as the basis. So, this is 84.3 kg. and how much molar mass will be obtained from it the molar mass is 12 kg per kmol. So, this will be 7.030 kmol. In the same way, you can extract N2 and O2. Where N2 is mentioned, the molar mass of nitrogen will be 28. When you remove this, NH2 will come out 0.945, 0.1375, 0.0225 and 0.0278 And all are in kilo mole. Now that you have it, you can write the reaction of it. Now, the air is because the one we were removing was of coal. Now, air is we will write it as A theoretical. I mean, we don't know how many kilomoles we need it. But theoretically, oxygen will come plus 3.76 nitrogen will come. And what will be in your reaction? CO2 plus Ys2O. Because it is sulfur, so sulfur dioxide will also be made SO2. plus, the nitrogen that has been released. Now you have to do elemental balance, mass balance. So, if you do mass balance, so we will do C, then H. So, what will be the result if we balance C? This is x here. So, x is on the right-hand side, 7.03 on the left. This is S2. S2 is here. So, y is here, simple 0.945. Then S is here, S is here. So S is here, z is equal to 0.027. 8 now what do you have N2 is there so if we see N2 and balance N2 so let's do O2 first let's balance O2 first if we do O2 it will be in left hand side 1.375 plus A S2 A T H means theoretical it will be in right hand side x plus 0.5 y, i.e. y by 2 plus z. So, we have taken this as well. So, from here, since we know x, y, z, theoretical comes out. Theoretical comes out to be 7.393. And then you will take out N2. In N2, in your left-hand side, 0.0225 plus 3.768 h. Here is W, so from here W came out, 27.82. so now you have all kinds of equations. All kinds of variables that you had to remove have been removed. Now, you can plug in again and write the complete equation. But what we have to remove is the mole fraction. Mole fraction. of the product gas. So, for this we have to take out the number of moles of CO2 divided by the total number of moles of the product. So, for this we have to take out N product. So, if we look at N product, what will be N product? If we look at N product, what will be N product? N product is the total number of moles of the system. So, this will be your x plus Normally, x plus y plus z plus W. So, this is 35.82 kilomoles. And what is your NCO2? NCO2 is 7.03, which is x. This is your x. This is x, right? This is your NCO2. So, this is 7.03 divided by kilomoles. Divided by 35.82 kilomoles. So, this is 0.1963 Right? 0.63 Similarly, you will get yS2 Similarly, you will get ySO2 Similarly, you will get yN2 So yS2O will be your NS2O divided by N product This is your 0.02638 ySO2 will be 0.000776 Yn2 will be 0.7767 So these are the total expressions of your mole fraction Now the question that we were asked is What is the apparent molar mass of the product gas? Now molar mass is or how much kg is in 1 kg mole. So, for molar mass, we have to find a simple expression. Molar m product is the mass of the product divided by moles of the product. So, if we have fixed moles of the product to be 35.82 kmol, then the question is how much mass is in it. So, there is nothing to do in it. So 7.03 mol x molar mass of CO2 will be multiplied Then y will be multiplied by molar mass of water And in the same way z will be multiplied by molar mass of SO2 And w will be multiplied by molar mass of N2 So the expression written here So 7.03 x 44 which is molar mass of CO2 Plus 0.945 molar mass of water plus 0.0278 molar mass of SO2 plus 27.82 molar mass of N2 so this is 30.9 kg per kilo mole now this is your molar mass now the last part was to extract air fuel ratio which is mass of air divided by mass of fuel Mass of air is 8 EH in theoretical unit 8 EH is 7.393 So A is 7.393 multiplied by 4.76 kgmol multiplied by 29 kg per kmol This is the air So 7.39 times 7.76 kilo mole into 29 kg per mole So this is divided by 100 kg So I will take this carefully 7.393 your ath multiplied by 4.76 We have taken the whole area which is kilo mole This is your total multiplied by 29 kg per kilo mole Okay divided by 100 kg which is 10.2 kg of air divided by 1 kg of fuel. So, now pay attention that this 10.2 kg which we had to supply to air per kg of mole, that is the ratio we have. We could have taken 1 kg of coal as a basis, but we have taken 100 because it is a very small number. So, we usually take 100 as a basis to make it easier to calculate.

Let's move ahead. Now we will do the next question on reverse combustion analysis. The question is that the octane is burned with dry air. There is no additional moisture in the burnt dry air. When it is burnt, it shows the composition but on a dry basis. It means that the water is not shown. So, this composition is on a dry basis. Look at the composition, it is 100% but the water is removed, and it is 100%. So, this is what we talked about, which gas analyzer are you using? This is Orsat gas analyzer which is used on a dry basis. Now the question is which has the air-fuel ratio and percentage of theoretical air used? You have to write the question on this. You can write the reaction on this. You can also take the basis of 100 kmol of product. Let's start. Let's understand how to write this. So, one important thing is that the analysis given is volumetric analysis. So, if we consider the product gas as ideal gas, then the volumetric fraction and the mole fraction will be equivalent in ideal gas. So, we will use this. And for this, we will consider it as mole fraction in the assumption of ideal gas. and that's why we will consider it as a 100 kilomole basis like the product. So, if we consider the product as a 100 kilo basis, then i can write the reaction. That C8H18, suppose it is X mol, in this your theoretical area O2 plus 3.76 N2 gives you 10.02 CO2 plus 5.6202 plus 0.88 CO plus 83.48 N2 plus the remaining water will be water because water will go but the composition is in the form of AF Now we have to find out X, A and B We have to find out X, A and B and for this we will do elemental balance and for that we will try to find out by doing elemental balance So first we will take N2 If we take N2, 3.76 times A, this came out from the left hand side, this is 83.48. So, from here A is 22.20. And then C is there. If we take C, then in the left-hand side, 8x is equal to 10.02 plus 0.88. So, this came out, your x is equal to 1.36. Then H is 18x and 2b is on the right-hand side so 2b is 12.24 then O2 is in the left-hand side and A is in the right hand side so 10.02 and 0.88 divided by 2 Then we have 5.62 and then we have b by 2. So, you can check the consistency of the equation. Because you have x, so on the left-hand side you have 22.20 and on the right-hand side you have 22.20. So, you can check the consistency of the equation. So, you don't need to use oxygen balance. You can find the three variables and equations. But you can check the consistency of the equation. So, finally you have this expression. Now, if we put this back, it will be in the form of X. So, X is 1.36 C8H18 plus 22.2. This is the other expression, and these are the other expressions. But if you write this on the basis of 1 kilomole of fuel, then you can divide 1.36 throughout. If we divide it, we get C18H18 plus 16.32 This is the area and 7.37 plus other things. So, this expression will come out. so, We can remove the tea if you want. Now, the question we had to answer after this was... that was the air-fuel ratio. For AF, you should have the amount of air. You have taken the basis of the fuel. So, you have taken 1 kmol of fuel, so 1 kmol is fixed, this will be the same. And air is 16.32 x 472 multiplied by molecular molar mass of air. So, this is your air mass. So, this is the mass of air, and this is the mass of fuel for 1 kmol of fuel. So, this is what we get. So, here it is 19.76 kg air per kg fuel. Now, we have to take out theoretical air. How much will it be? For theoretical air, we can assume that it is completely combustion. So, we will use 1 mole of C8H8 fuel. So, we will use 1 C8H8 fuel for 1 kmol. And we have to extract 8 . This is air. and it is completely combustion 8CO2 will be formed, 9H2 will be formed plus 3.76 times ath will be the net which will be inert from here you get the value of ath 12.5, so this is theoretical you wrote the equation again properly completed the combustion according to that the value of ath will be obtained by the balance of the elements Now, if your ath is 12.5, you can calculate the percentage of theoretical air. Your actual air is Nm, which is Nm. So, NM air actual divided by NM air theoretical. M is common, it will be cancelled. So, the actual number of moles of air, the number of moles of air theoretical This will be per kmol of the fuel. So, per kmol, 16.32 was your number of moles. So, this is your number of moles divided by 12.5. So, this is 131%. So, from here, this 4.76 will be cancelled. So, only 16.32 divided by 12.50 will remain. and according to that you will get 131% So I hope you understood how we have done this analysis The only important assumption is that according to the volumetric analysis we have given you we have said that according to the ideal gas you can write the volumetric fractions in the form of mole fraction and that is why you have assumed it in the form of mole fraction and then took the basis and then you can assume it, expand it and then you can get the values and then the rest of the scaling you did from 1.36 you got per unit kilomole and then you did the rest of the calculations based on the formula to show theoretical error you again showed the equation which is fully combustion and from there you can The amount of theoretical moles is calculated. The percentage of theoretical moles is actually divided by the number of moles of theoretical moles for 1 kilomole of fuel. So, according to this, 131% is calculated. So, let's stop here in this lecture. In the next lecture, we will understand about enthalpy and other things, particularly adiabatic flame temperature. So, let's meet again in the next lecture. Till then, bye-bye.