Engineering Thermodynamics
Professor Jayant K Singh
Indian Institute of Technology Kanpur
Department of Chemical Engineering
Module 8
Lecture No 56
Energy balances for reacting systems

Welcome back uh, so we were discussing the chemical reaction and in the last lecture we went through the definition of air fuel ratio and as well as described some examples of the types of fuel ok. We have also discussed that the moles are not balanced it is a conservation of mass balance which we are going to use in order to analyse the chemical reactions for commercial processes ok.

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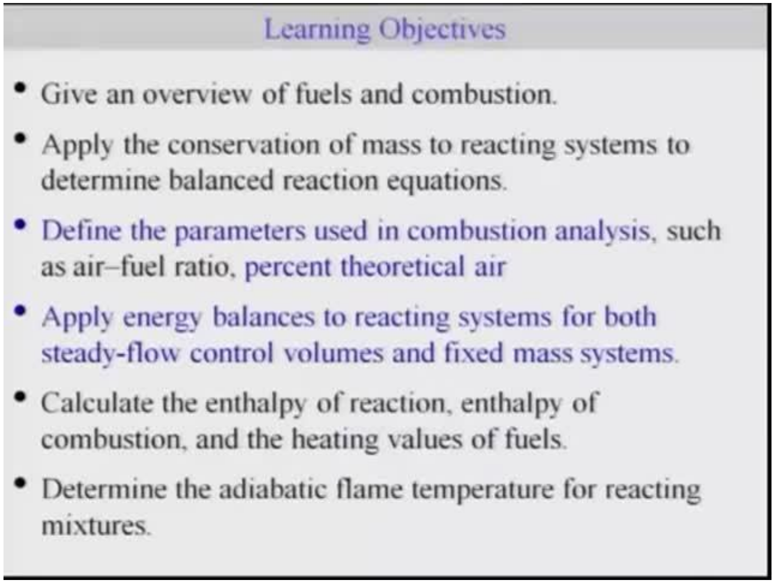

Learning Objectives

- Give an overview of fuels and combustion.
- Apply the conservation of mass to reacting systems to determine balanced reaction equations.
- Define the parameters used in combustion analysis, such as air–fuel ratio, percent theoretical air
- Apply energy balances to reacting systems for both steady-flow control volumes and fixed mass systems.
- Calculate the enthalpy of reaction, enthalpy of combustion, and the heating values of fuels.
- Determine the adiabatic flame temperature for reacting mixtures.

So in this lecture I will continue that discussion and present some of the combustion analysis particularly the percentage of theoretical air and we will try to do some energy balance for acting some system for both study flow control volume and fixed mass system ok. As we realised in our basic analysis that there is a possibility of that some of the combustion cannot lead to the completion due to for example if the air is not sufficient or there is a possibility that you know excess air is given. So if the combustion is complete but you still have some of the air left in the product stream.

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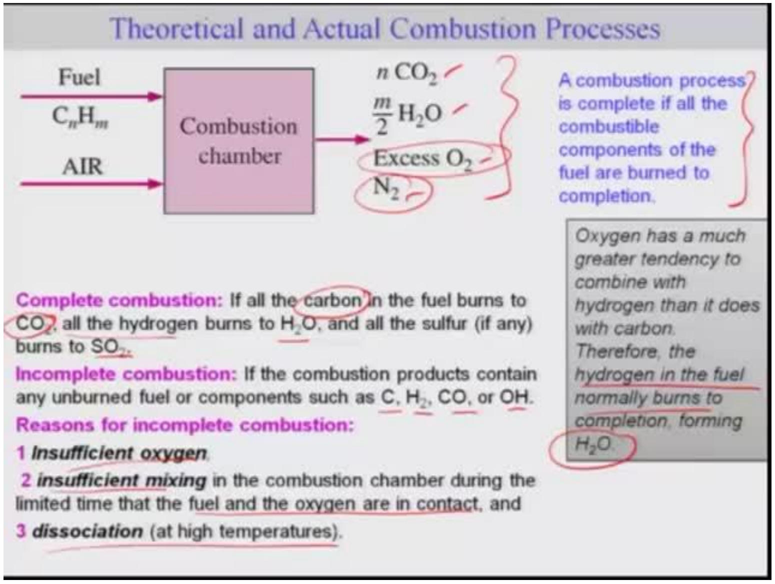

Theoretical and Actual Combustion Processes

Fuel C_nH_m

AIR

Combustion chamber

$n\,CO_2$

$\frac{m}{2}H_2O$

Excess O_2

N_2

A combustion process is complete if all the combustible components of the fuel are burned to completion.

Oxygen has a much greater tendency to combine with hydrogen than it does with carbon. Therefore, the hydrogen in the fuel normally burns to completion, forming H_2O.

Complete combustion: If all the carbon in the fuel burns to CO_2, all the hydrogen burns to H_2O, and all the sulfur (if any) burns to SO_2.

Incomplete combustion: If the combustion products contain any unburned fuel or components such as C, H_2, CO, or OH.

Reasons for incomplete combustion:

1 ***Insufficient oxygen***

2 ***insufficient mixing*** in the combustion chamber during the limited time that the fuel and the oxygen are in contact, and

3 ***dissociation*** (at high temperatures).

So combustion process is complete only if the combustible components of the fuel are burnt to completion ok, so this is kind of a theoretical experiment ok and many times you may have to provide little more because you may not know exactly the the contents of the fuels or you would like that absolutely the fuel should be burnt, so hence we need to add more fuel in order to add more oxidise or air in order to have complete combustion ok.

So there is a theoretical limit, so we call it a theoretical air percentage, so let me just go through that, so this is an example of let us say fuel and air leading to CO2, S2, O2 and N2 ok, so this is a typical kind of product which will form when you burn hydro carbon fuel ok. So as I said air could be in excess and hence you may have stream not just a inert components such as the nitrogen but excess oxygen also along with CO2 and H2O as a final product ok.

Now oxygen has a much greater tendency to combine with hydrogen than it does with the carbon and therefore usually you will see after the completion of the combustion you may, you will be you know the product will contain mainly S2O plus a CO2. So thus the hydrogen in the fuel normally burns to completion forming H2O ok, so this is more possibilities beside of course forming CO2.

Let me just go through the definition of complete and in complete combustion So the complete combustion is if all the carbon in the fuel burns to CO2 ok, so that is that means CO2 has to be present and all the hydrogen burns to H2O and all the sulphur, if any burns to SO2 ok. Now we are quite well aware the SO2 and CO2 are not so good for environment ok but this is something which also relies that we reduction in the carbon in the fuel and sulphur in the fuel is critical to have better fuel for or the more environmentally fuel ok.

Now if there is incomplete combustion, then the combustion product contains components such as CH2CO and OH ok. So what are the reason for incomplete combustion? Of course the first is that you do not have sufficient air or sufficient oxidiser, so that means insufficient oxygen ok. Another possibility would be that insufficient mixing maybe present in the combustion chamber which during the limited time fuel and oxygen are in contact.

So if you do not allow fuel and oxygen to to have a proper contact, that means the time is limited and hence it does not mix well and it does not burn. So this is another possibility, the other other possibility could be that it temperature could be a very very high and the combustion chamber leading to dissociation ok and thus it will not go through the regular mechanism of reaction ok.

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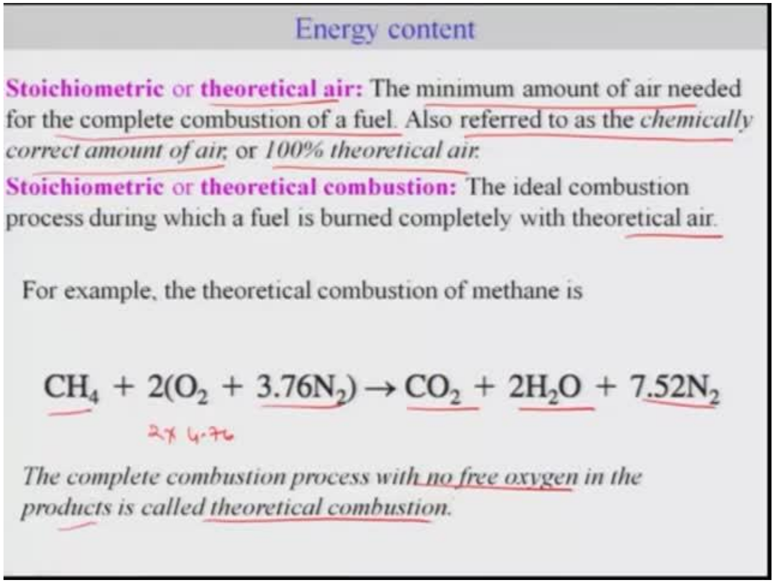

Energy content

Stoichiometric or **theoretical air:** The minimum amount of air needed for the complete combustion of a fuel. Also referred to as the *chemically correct amount of air,* or *100% theoretical air.*

Stoichiometric or **theoretical combustion:** The ideal combustion process during which a fuel is burned completely with theoretical air.

For example, the theoretical combustion of methane is

$$CH_4 + \underset{2 \times 4.76}{2(O_2 + 3.76N_2)} \rightarrow CO_2 + 2H_2O + 7.52N_2$$

The complete combustion process with no free oxygen in the products is called theoretical combustion.

So there is a certain theoretical limit for the complete combustion and one can do a simple reaction balance here or elemental balance and try to get the theoretical estimate of the AF which is required for 100 percent combustion of the fuel. So this is what we define as the theoretical air or sometimes also called stoichiometric air which is the minimum amount of air need for the complete combustion of the fuel ok, so it is also referred to as a chemically correct amount of air or 100 percent theoretical air. So the stoichiometric or theoretical combustion is the ideal combustion process during which a fuel is burnt completely with the theoretical air.

So this is an example of combustion of methane, so methane takes like one mole of methane will take 2 moles of oxygen leading to complete combustion of CO2, H2 water, whatever remains in it will be will come out as it ok. So this is the complete combustion with no free oxygen in the product ok and the thus this is also a theoretical combustion. So that means the theoretical air here is nothing but some 2 into you know 4.76 kilo mole of air, so that is something which we would call theoretical air.

This becomes a kind of a limit or kind of a criteria for which we can you know add additional amount of air in terms of excess ok in order to have surety that you know the combustion will lead to completion ok.

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That is we define other terms such as you excess air which is the amount of air in excess of this Trico metric amount and usually this referred in terms of percentage excess air or percentage theoretical air ok. So all deficiency of air which is the amount of air less than the stoichiometric amount of an express as a percentage deficiency of air. Equivalence ratio though it is not very commonly used is the ratio of the actual fuel air ratio to the stoichiometric fuel air ratio ok.

So this is an example of typical way of using this access air or theoretical air, so if somebody says that 50 percent access air ok, it means nothing but the theoretical air plus 50 of the theoretical air which means that this is nothing but 150 percent of the theoretical air ok. So this is nothing but your theoretical air plus 50 percent of which is nothing but 150 percent of theoretical air. So 200 percent of excess air is nothing but of course the same logic is a 300 percent theoretical air, 90 percent of theoretical air is 10 percent deficiency of air ok. So this is the different terminology which we are going to make use of it in our analysis ok.

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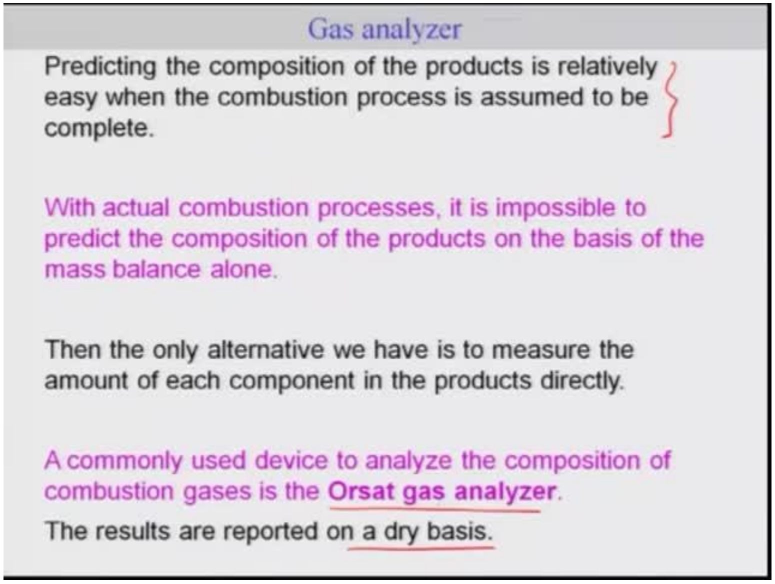

Gas analyzer

Predicting the composition of the products is relatively easy when the combustion process is assumed to be complete.

With actual combustion processes, it is impossible to predict the composition of the products on the basis of the mass balance alone.

Then the only alternative we have is to measure the amount of each component in the products directly.

A commonly used device to analyze the composition of combustion gases is the **Orsat gas analyzer**.

The results are reported on a dry basis.

Now how do you find or analyse the product of the combustion? Ok, so this is something which is important in order to see it the combustion is complete ok and thus this is a kind of a critical part of your combustion reaction to analyse the gases which are formed in product. So predicting the composition of gas product is relatively easy ok when the combustion process is assumed to be complete. However it is not possible to predict the composition of the product on the basis of mass balance alone with actual combustion process.

So then the only alternative we have is to measure them amount, so what we are trying to say is that many a times it is not feasible to assume that the combustion is is complete and thus is critical that you analyse the product gas composition. Now this particular analysis is typically done by something called Orsat gas analyser ok which are reported on a dry bases that means the water is not considered in the analysis of it ok that is the meaning of the dry bases ok.

So we will be assuming that the composition which we have been given is either through Orsat gas analyser in general ok. So whether it is a dry bases or wet bases that something which would be provided to us.

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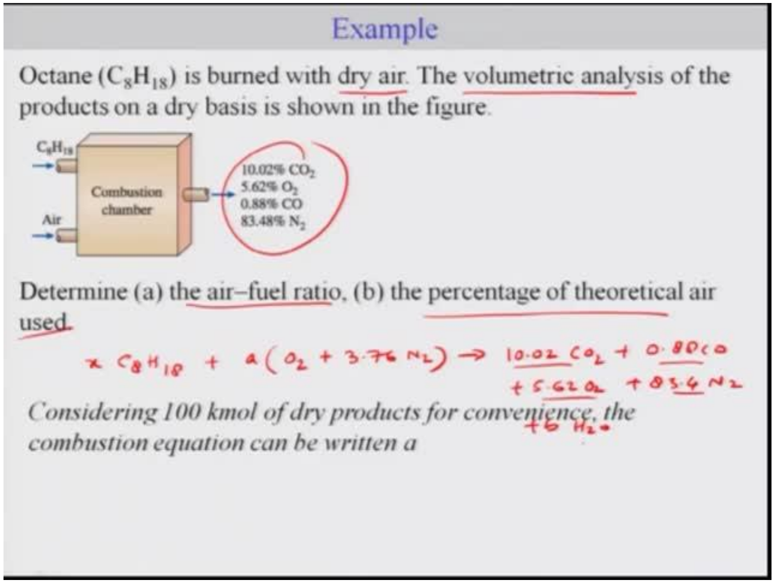

Example

Octane (C_8H_{18}) is burned with dry air. The volumetric analysis of the products on a dry basis is shown in the figure.

Determine (a) the air–fuel ratio, (b) the percentage of theoretical air used.

$$x\, C_8H_{18} + a(O_2 + 3.76 N_2) \rightarrow 10.02\, CO_2 + 0.88\, CO + 5.62\, O_2 + 83.4\, N_2 + b\, H_2O$$

Considering 100 kmol of dry products for convenience, the combustion equation can be written a

So this is an example ok. Here the octane is burnt with dry air which essentially means it does not contain any moisture and this is the analyser volumetric analysis of the product on a dry bases of course so using some kind of analyser such as your Orsat gas analyser and what we need to find is the air fuel ratio and the percentage of theoretical air used ok. And other thing which we have to calculate is the percentage of theoretical air used, so let me start with basic equation here, so of the combustion of octane.

It is not being mentioned that the amount of octane which is being burnt ok, what we know is the composition of the product first of all but that also with a dry air. We should also assume that there is a water because as we know the hydrogen will burn completely leading to water in the product, that means we need to write something like this that you have octane, let us assume that you have X mole of octane, this is burnt with certain mole of oxygen that is oxygen plus nitrogen, so this is the A mole of it, leading to this is volumetric analysis, so we are on a dry bases, so let us assume this as 10.02, CO2 plus 0.88 CO and some amount of water ok.

So now we have this equation where lot of unknowns are there and the only way we can solve this problem is by doing a mass balance of each element ok. So let us assume that there is a, so what we have done in this case of course is we have assumed that a 100 kilo moles of dry product is used. That is why we can clearly write this as as the number of moles for product for the dry products ok.

Then of course we do not know about the water thus we have written the moles of water being also as a part of the product.

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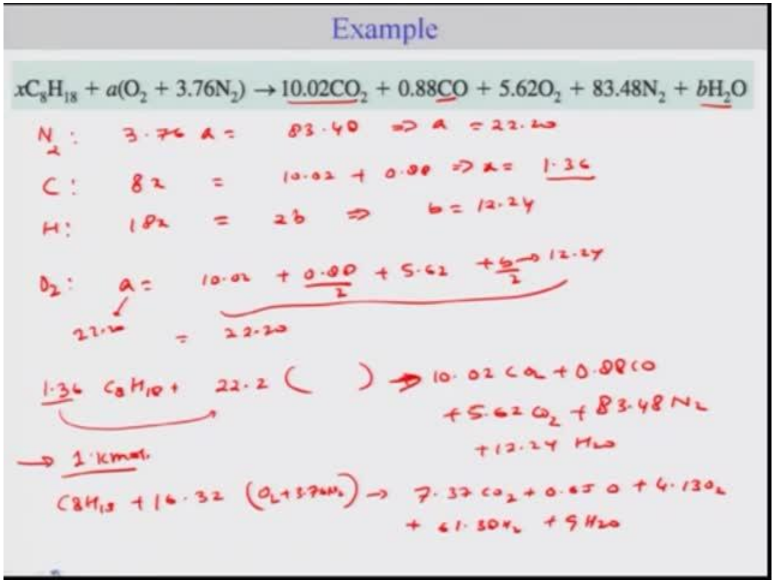

Example

$xC_8H_{18} + a(O_2 + 3.76N_2) \rightarrow \underline{10.02CO_2} + 0.88\underline{CO} + 5.62O_2 + 83.48N_2 + b\underline{H_2O}$

N_2 : $3.76a = 83.40 \Rightarrow a = 22.20$

C : $8x = 10.02 + 0.88 \Rightarrow x = \underline{1.36}$

H : $18x = 2b \Rightarrow b = 12.24$

O_2 : $\underset{22.20}{a} = \underbrace{10.02 + \frac{0.88}{2} + 5.62 + \frac{b}{2}}$ → 12.24

22.20 = 22.20

$\underline{1.36}\ C_8H_{18} + 22.2(\quad) \rightarrow 10.02CO_2 + 0.88CO$
$+ 5.62O_2 + 83.48N_2$
$+ 12.24H_2O$

→ $\underline{1\ \text{kmol.}}$

$C_8H_{18} + 16.32(O_2 + 3.76N_2) \rightarrow 7.37CO_2 + 0.65O + 4.13O_2$
$+ 61.30N_2 + 9H_2O$

Ok, so we have this equation, now what we can do is, we can write mass balance for individual components ok, so let us write this is for nitrogen to start with ok considering N2 rather than N 3.76 is on the left side multiplied by A, this should be equal to 83.48 leading to A is 22.20 ok. What about carbon? 8X is 10.02 which is from here plus point 88 for carbon mono oxide leading to excess 1.36. Then you have 18CX is equal to 2, 18X equals to B, B is 12.2 ok.

Now at this point you have all the values of AXB, you can also verify whether this is correct by doing a analysis O2. O2 is A should be equal to 10.02 plus 0.88 divided by 2 plus 5.62 plus B by 2 and indeed this is your 22.20, this is your 12.24 and if you do this, this summation of these individual terms, this turns out to be 22.20 which is means that you have done it correctly.

Ok, so you have now X which is 1.36, you can write this X in terms of 1.36 C8 H18 plus A is your 12.24 ok plus 10 point, so this gives you 10.02 CO2 ok, so this I can write here and this will become B is your 12.24 H2O, now you can convert this thing to kilo mole as bases ok for C8 H18, this becomes C8 H18 plus 16, this is your A, so this should have been your 22.2 ok. So when you divide this, this number by this number in order to get bases for 1 kilo mole for octane, this becomes 16.32 ok which is nothing but O2 plus 3.76 and 2 and this is your 7.3702 ok.

So this becomes your bases for with respect to your 1 kilo mole bases ok. Ok, so what we have done till now is obtained this complete equation for 1 kilo mole of octane, so this is chemical reaction for the combustion of octane and corresponding to this, you have theoretical air as well ok.

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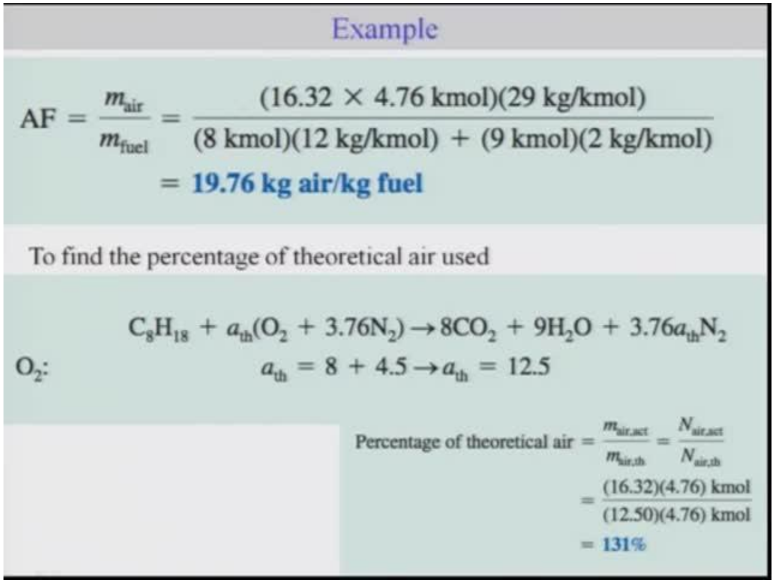

Example

$$AF = \frac{m_{air}}{m_{fuel}} = \frac{(16.32 \times 4.76\ \text{kmol})(29\ \text{kg/kmol})}{(8\ \text{kmol})(12\ \text{kg/kmol}) + (9\ \text{kmol})(2\ \text{kg/kmol})}$$

$$= \mathbf{19.76\ kg\ air/kg\ fuel}$$

To find the percentage of theoretical air used

$$C_8H_{18} + a_{th}(O_2 + 3.76N_2) \rightarrow 8CO_2 + 9H_2O + 3.76a_{th}N_2$$

$$O_2: \quad a_{th} = 8 + 4.5 \rightarrow a_{th} = 12.5$$

$$\text{Percentage of theoretical air} = \frac{m_{air,act}}{m_{air,th}} = \frac{N_{air,act}}{N_{air,th}}$$

$$= \frac{(16.32)(4.76)\ \text{kmol}}{(12.50)(4.76)\ \text{kmol}}$$

$$= \mathbf{131\%}$$

So look at the problem, the first thing which we wanted to know is air fuel ratio, ok so we already know the mass of the air ok because with respect to 1 kilo mole bases we have already written the equation here, so this is equation that means your M air is 16.32 into 4.76 kilo mole because that is including the oxygen and nitrogen and multiplied by the mole of mass of air, fuel is 8 kilo mole multiplied for the carbon and then for hydrogen so that makes your air fuel ratio is 19.76 kilo kg air divided by or per kg fuel, so 19.76 kg air per kg fuel.

Now the next question is to find the percentage of theoretical air which we have to use. So theoretical air is on the bases of for the fact that you have complete combustion ok, thus you need to write this equation, one kilo mole of C8 H18 plus A A kilo moles of air leading to 8CO2 plus 9H2O plus the inner part ok. And from here you can get the theoretical moles of air which gives you 12.5 by using simply the elemental or the mass balance of air.

So this becomes your theoretical air to be used and thus you can find out the percent of theoretical air which is nothing but mass of the actual air divided by mass of the theoretical air and what is the mass of the actual air which is nothing but your 16.32 kilo moles ok.5 So 16.32 kilo moles multiplied by of course the oxygen plus nitrogen that means 4.76 kilo, so this is the total kilo moles of air and this 12 point particular limit ok multiply 4.76 and this gives you 131 percentage.

So thus in the previous combustion example we used 131 percentage of theoretical air or in another word uh, in other word 31 percent excess air we have used in order to have this combustion process for the octane ok.

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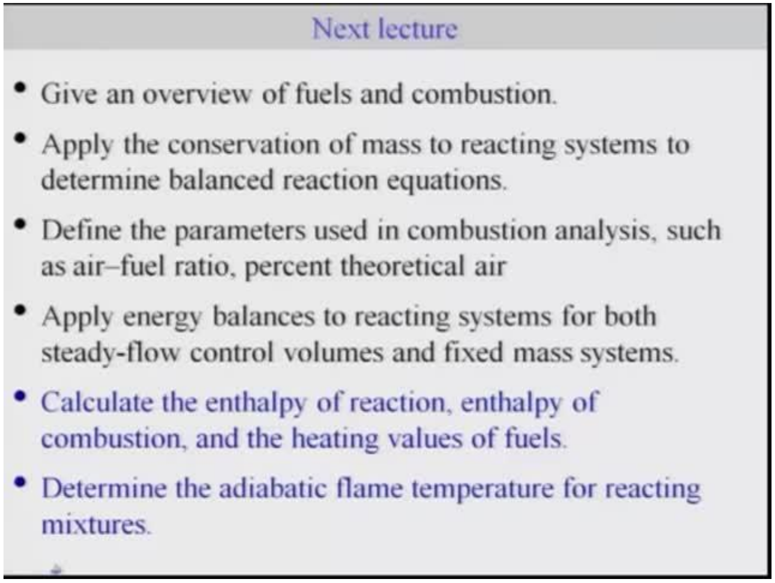

Next lecture

- Give an overview of fuels and combustion.
- Apply the conservation of mass to reacting systems to determine balanced reaction equations.
- Define the parameters used in combustion analysis, such as air–fuel ratio, percent theoretical air
- Apply energy balances to reacting systems for both steady-flow control volumes and fixed mass systems.
- Calculate the enthalpy of reaction, enthalpy of combustion, and the heating values of fuels.
- Determine the adiabatic flame temperature for reacting mixtures.

So I hope this particular example illustrates how to make use of elemental balances in order to find the theoretical air or excess air or percentage of excess air ok. So that will be the end of this particular lecture, in next lecture we will take up enthalpy balances and other aspect of energy balance related to chemical reactions ok. See you in the next lecture.