

Engineering Thermodynamics
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Module 8
Lecture No 55

Combustion and conservation of mass in a chemical reaction

Ok welcome back uh, we are going to start a new topic. It is on chemical reaction which is a very integral part of thermodynamics in industrial scale, particularly where the thermal energy is being generated using some kind of reaction fuel burning leading to generation of energy.

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Learning Objectives

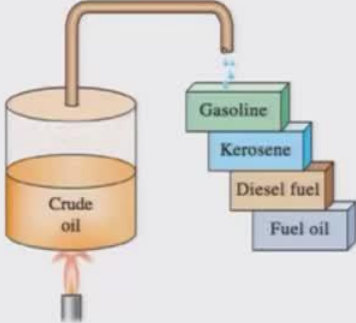
- Give an overview of fuels and combustion.
- Apply the conservation of mass to reacting systems to determine balanced reaction equations.
- Define the parameters used in combustion analysis, such as air-fuel ratio, percent theoretical air
- Apply energy balances to reacting systems for both steady-flow 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.

Fuel and Combustion

Fuel: Any material that can be burned to release thermal energy.
Most familiar fuels consist primarily of hydrogen and carbon. They are called **hydrocarbon fuels** and are denoted by the general formula C_nH_m .

Hydrocarbon fuels exist in all phases, some examples being coal, gasoline (usually treated as octane C_8H_{18}), and natural gas.

Most liquid hydrocarbon fuels are obtained from crude oil by distillation.



The diagram illustrates the distillation of crude oil. A cylindrical container labeled 'Crude oil' is shown with a flame underneath it, indicating it is being heated. A pipe extends from the top of the container to a distillation column. The column is represented by a series of four stacked rectangular boxes, each representing a different fuel fraction: 'Gasoline' (top), 'Kerosene', 'Diesel fuel', and 'Fuel oil' (bottom). The diagram shows the separation of these different fuel types based on their boiling points.

So this is what the overview of this particular topic uh. I will start with the definition of fuel and combustion. Fuel is basically any material that can be burned to release the thermal energy. The most common fuel consist of primary hydrogen and carbon in terms of hydro carbon which is a commonly known fuel and its general formula is C_nH_{2n+2} ok. Now typical destination column or the separation of the crude oil which separate based on the density for example is restated in this form where different types of fuel is separated, such as gasoline, kerosene, diesel oil, diesel fuel, fuel oil, these are all hydro carbon fuels which exist in different phases, normal conditions, some in gas phase, some in solid phase ok depending on the densities.

The most common hydro fuel is basically octane for example ok and natural gas for example is another one which consist of mainly methane ok. Now in addition one can have other kind of hydro common fuel which are consist of methyl alcohol or methanol ok which is commonly also used now days in different existing fuel to create some kind of blended fuel and this is mainly because to reduce the content of CO_2 in the atmosphere or in other word to make it more environmentally friendly.

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Energy content

Alternative fuels is now in demand which are friendlier to the environment such as natural gas, alcohols (ethanol and methanol), liquefied petroleum gas (LPG), and hydrogen

TABLE 15-1
A comparison of some alternative fuels to the traditional petroleum-based fuels used in transportation

Fuel	Energy content kJ/L	Gasoline equivalence,* L/L-gasoline
Gasoline	31,850	1
Light diesel	33,170	0.96
Heavy diesel	35,800	0.89
LPG (Liquefied petroleum gas, primarily propane)	23,410	1.36
Ethanol (or ethyl alcohol)	29,420	1.08
Methanol (or methyl alcohol)	18,210	1.75
CNG (Compressed natural gas, primarily methane, at 200 atm)	8,080	3.94
LNG (Liquefied natural gas, primarily methane)	20,490	1.55

* Amount of fuel whose energy content is equal to the energy content of 1-L gasoline.

And thus these new alternative fuels are becoming more important, increasingly important in current usage in industry as well as in automobile industry ok and thus we need a friendly fuels for the environment and importance of natural gas, alcohol, LPG's hydrogen is becoming increasingly important.

Now one can look at this table which provides energy content of different kind of fuel considering gasoline as the bases for the energy content and one can clearly see is that your LPG's, ethanol, CNG's these are high energy content and thus is also useful that you will burn same amount of mass but obtain much higher amount of energy based on this particular table illustrates that. And thus it is becoming quite relevant to make use of such kind of fuels in daily usage.

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Combustion

Combustion

- A chemical reaction during which a fuel is oxidized and a large quantity of energy is released is called **combustion**.
- The oxidizer most often used in combustion processes is air
- O₂ is used as an oxidizer only in some specialized applications, such as cutting and welding, where air cannot be used

Air
(21% O₂
79% N₂)
1 kmol O₂
3.76 kmol N₂

1 kmol O₂ + 3.76 kmol N₂ = 4.76 kmol air

Combustion of air

- Nitrogen behaves as an **inert gas**.
- Nitrogen usually enters a combustion chamber in large quantities at low temperatures and exits at considerably higher temperatures, absorbing a large proportion of the chemical energy released during combustion.

Ok, so one of the primary thing which primary physics behind the this energy generation is combustion and thus we need to little bit spend some time on it. combustion is nothing but a chemical reaction ok, during which fuel which we already discussed different kind of fuel is oxidised and a large quantity of energy is being generated, so this is basically combustion and thus we need an oxidiser which is merely air.

But in many cases oxidiser would be a pure O₂ such as used in cutting and welding ok, air will contain not only oxygen but as well as nitrogen ok, so if we consider one kilo mole of oxygen, the cost burning number of moles of nitrogen is 3.76 and thus the total amount of air would be 4.76 kilo mole ok. Nitrogen acts like inert. Ok we will be assuming that basically it behaves more like a inert gas and thus it will enter as a react as well as a reactant or in a reactant space but as well as it will exit in the product phase as nitrogen oxide.

So though it acts like an inert gas but it will effect the outcome of the combustion ok because it enters typically at low temperature but exist at considerably at high temperature ok and thus it absorbs large portion of the chemical energy which is being released during the combustion ok, thus it will also effect the outcome of the combustion.

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Conservation of mass during a chemical reaction

$$C + O_2 \rightarrow CO_2$$

$$m = NM$$

m mass
N number of moles
M molar mass

The total number of moles is not conserved during a chemical reaction.

Chemical equations are balanced on the basis of the conservation of mass principle (or the mass balance), which can be stated as follows: The total mass of each element is conserved during a chemical reaction

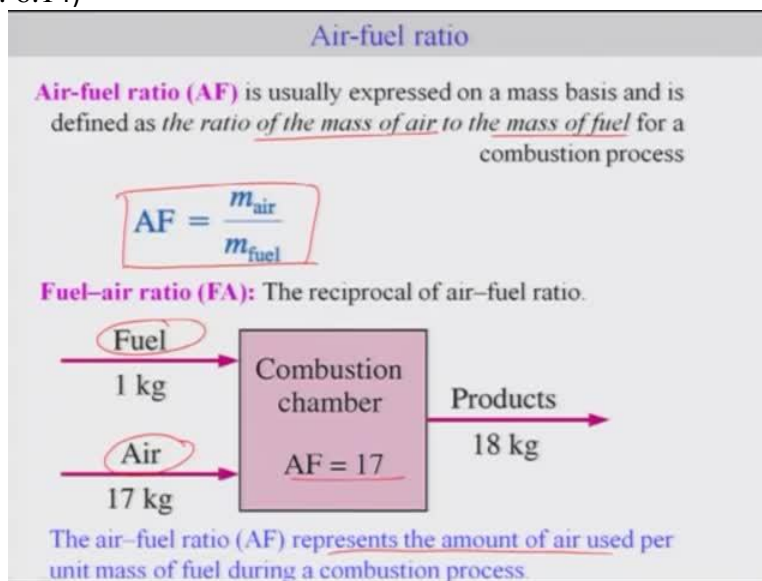
Ok, so let me go through a bit of the mass balance or an so one can clearly see based on little bit of exercise that the moles are not going to be balanced with the chemical reaction, it is only the mass of the elements which are going to be balanced, take an example of generation or formation of a carbon dioxide from a simple carbon element and oxygen will lead into CO₂ thus you have one mole of carbon plus one mole of oxygen leading to one mole of CO₂. Clearly one can see that moles are not balanced.

On the other hand the mass of individual elements are balanced which one can see here ok. Now mass is connected to the number of mole and the molar mass from this expression ok? The chemical equations are balanced of the bases of the conservation of the mass principle or the mass balance ok which we state as follows- The total mass of each element is conserved during a chemical reaction. For example in the case of water formation from hydrogen oxygen, 2 kg of water plus 16 kg of oxygen leads to 2 kg of hydrogen and 16 kg of oxygen which is part of the water ok.

Though the number of moles are different because here it is one mole and this is half mole ok leading to one mole of water. So in this case we need to balance hydrogen which should be balanced and as well as oxygen. So clearly the reactant which is this contains 2 kg of hydrogen and oxygen 16 kg and as well as this would be the same for the product case ok as you can clearly see from the water.

So that is how we are going to make use of it in the, in the analysis as well, later on we will clearly use this mass balance for our analysis ok.

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Now the fuel automatically does not burn by itself and this is good otherwise it will be burning all the time uh. So it requires a certain kind of a temperature at which it will start igniting itself ok and this is what we call it ignition temperature ok. So ignition temperature is the temperature which is a minimum temperature at which the combustion occurs for a fuel, so for example for gasoline it is 260 degree Celsius, carbon 400 degree Celsius, hydrogen 580 degree Celsius, carbon monoxide 610 degree Celsius and 630 degree Celsius for methane ok.

In addition to this you need a sufficient amount of oxidiser or for example air for burning of fuel. So a proportion of the fuel and air must be in a proper range for combustion to begin. For example natural gas does not burn in air in concentration less than 5 percent or greater than about 15 percent, so this is something it is quite relevant that there is a certain range of oxidise or air

which is required in order to burn the fuel ok or in order to combustion to occur. So which means there is a certain air fuel ratio which is necessary.

So let us first define what is air fuel ratio? So the air fuel ratio is nothing but the ratio of the mass of air to the mass of fuel, so it is defined on the basis of mass, so AF is an acronym for air fuel ratio is nothing but MA air divided by M fuel ok, for example this is the fuel the as a reactant and air ok, this is reactant leading to combustion or in combustion chamber leading to product, so in this case the air fuel ratio is nothing but 17 is like 17 kg of air divided by 1 kg of fuel ok.

The reciprocal of air fuel ratio is fuel air ratio ok, so this is sometimes used but most commonly used is AF ratio. So the air fuel ratio represent the amount of air used per unit mass of fuel during a combustion process. So this is sometimes a terminology which use in order to solve the problem.

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Balancing the combustion equation

One kmol of octane (C_8H_{18}) is burned with air that contains 20 kmol of O_2 , as shown in Figure below. Assuming the products contain only CO_2 , H_2O , O_2 , and N_2 , determine the mole number of each gas in the products and the air-fuel ratio for this combustion process.

$1 C_8H_{18} + 20 (O_2 + 3.76 N_2)$
 $\rightarrow 2 CO_2 + y H_2O + 20 O_2 + w N_2$

Mass bal. (atom by atom)

C: $8 = 2 \Rightarrow 2 = 4$

H: $18 = 2y \Rightarrow y = 9$

O: $20 \times 2 = 2 \times 2 + y + 2z \Rightarrow z = 7.5$

N_2 : $20 \times (3.76) = w \Rightarrow w = 75.2$
 $(w) = 20 \times 3.76 = 75.2$

So let us take an example to find out the number of moles for each gas and as well as the air fuel ratio for the combustion chambers, so this is an example of 1 kilo mole of octane which is burned with air ok, so this contains 20 kilo mole of O_2 assuming that the product contains only CO_2 , H_2O , O_2 , N_2 determine the mole number of each gas in the product and the AF ratio for this combustion process.

So the first thing what we are going to do is to write the chemical reaction of the equation here. So octane is C_8H_{18} , it is already assumed to be 1 mole, so this becomes 1 ok. So basically it is nothing but 1 into C_8H_{18} plus 20 kilo mole of air, so air contains O_2 plus 3.76 of nitrogen, so I am going to write here 20 which is being multiplied here. This leads to product spaces and we don't know the moles of those this products.

So hence we are going to use whatever is written here X, Y, Z, so $X CO_2$ plus $Y H_2O$ plus $Z O_2$ plus W ($9:40$) ok. Now we know that the mole are not going to be balanced so the first thing is to do a mass balance of each spaces ok? So let me start the exercise here, so the mass balance or you can also make use of total number of atoms. Ok it is the same thing because the molar mass will get cancelled among the right hand side and right left hand side of the equation, so one can do simple total number of more atoms instead of writing the complete mass balance.

So for example, so I can write 8 this multiplied because there are 8 atoms, this multiplied by its atomic mass is equal to X multiplied by atomic mass, the atomic mass will get cancelled so simply 8 is nothing but X ok. Similarly I can write for H 18 hydrogen atoms should be equal to hydrogen is here only in water, so this becomes your 2 times Y, so this means Y is nothing but 9 ok, X is nothing but 8 and then you have this O oxygen, oxygen on the left hand side is 20 times 2 these many atoms, this should be 2 times X plus Y plus Z into 2 ok.

And if you plug these values you can get Z as 7.5 ok, similarly N_2 is 20 times 2 and 3.7 here so you, either you can write N_2 , if you are writing N_2 then I should erase, I should erase this because this is only the balance of N_2 ok not N but it would be more or less same or it is it will give the same eh results and this should equal to W. Ok, I can also write this for N is equivalent 20 into 2 3.76 into W, so this is equivalent to this expression and this is $WS 75.2$ ok.

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$$AF = \frac{m_{air}}{m_{fuel}} \quad m \rightarrow (N \cdot M)$$
$$= \frac{(NM)_{air}}{(NM)_C + (NM)_H} = \frac{(20 \times 4.76) (29 \text{ kg/kmol})}{(8 \text{ kmol}) \left(\frac{12 \text{ kg}}{\text{kmol}} \right) + (9 \text{ kmol}) \left(\frac{2 \text{ kg}}{\text{kmol}} \right)}$$
$$= 24.2 \text{ kg air / kg fuel}$$

i.e. 24.2 kg air is used to burn each kg of fuel during this combustion process

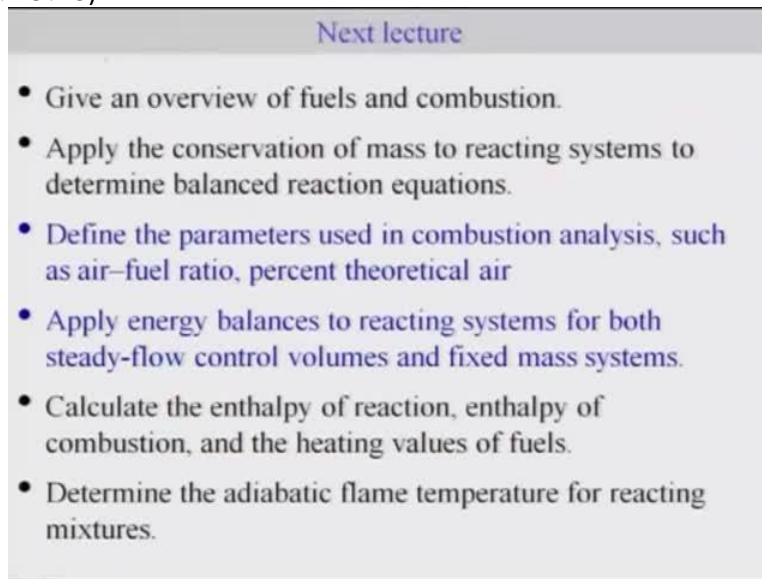
Now I can write down the air fuel ratio which is nothing but M air by M fuel, ok the mass is nothing but your N number of moles multiplied by molar mass, so this can be written as NM for air and for the case of fuel, now fuel consist of carbon and hydrogen ok, so I can write NM of carbon plus NM of a hydrogen which can further be written as the number of moles for air is 20 into 4.76 that will be total number of kilo moles ok multiplied by 29 kg, per kg mole ok, kg mole here divided by the number of kilo moles for carbon is going to be 8 only ok.

So because the number of carbons are 8, so we are taking 1 kilo mole as a bases for the fuel, so that becomes total number of moles for kilo for carbon it is going to be 8 kilo mole corresponds to 12 kg per kilo mole ok and similarly for hydrogen, for hydrogen is going to be your 18, so 18 is a hydrogen atom but for H₂ ok is going to be 9 correspondingly 9, 9 kilo mole, you can also write the same expression for hydrogen atom instead of H₂, so 9 kilo mole multiplied by 2 kg per kilo mole ok. So this gives us 24.2 kg of air per kg of fuel. ok that is your air fuel ratio.

So this means that 24.2 kg of air is used to burn each kg of fuel during this combustion ok process. Ok, so that way what we have done, we have determined the moles and this was determined by calculating the balance by performing the mass balance for each individual elements and leading to this number of moles for the product streams, product spaces. In addition we also calculate the air fuel ratio.

So this is a simple exercise to illustrate how to go about solving such problems ok.

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Next lecture

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- Calculate the enthalpy of reaction, enthalpy of combustion, and the heating values of fuels.
- Determine the adiabatic flame temperature for reacting mixtures.

So that will be the end of this particular lecture, in the next lecture I am going to describe a bit of combustion analysis and as well as some to for the reacting systems for both solid state and fixed mass systems ok. So see you in the next lecture.