

Fundamentals of Combustion
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Lecture – 01
Fuel and their Properties – Part 1

This course is called Fundamentals of Combustion and this is a fundamental course which can be core or elective depending upon the curriculum. This covers the basic aspects of combustion. We will basically spend say about 36 hours of lectures in this including tutorials and small quizzes and so on.

Basically, we will be able to cover lot of aspects of thermodynamics, stoichiometry and so on, let us see that. I am Professor V. Raghavan, from the Department of Mechanical Engineering, Indian Institute of Technology, Madras.

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Course Contents



- (1) Fuels and their properties
- (2) Review of basic thermodynamics of ideal gas mixtures
- (3) Stoichiometry
- (4) First and Second Laws of Thermodynamics applied to combustion;
Heat, temperature and composition of products in equilibrium
- (5) Mass transfer basics
- (6) Fundamentals of combustion kinetics
- (7) Governing equations for a reacting flow
- (8) General characteristics of combustion flame and detonation
- (9) Laminar flame propagation-Flammability limits and quenching of
laminar flames-Ignition-Flame stabilization
- (10) Gas jets and combustion of gaseous fuel jets
- (11) Turbulent premixed and non-premixed flames
- (12) Droplet evaporation and combustion
- (13) Combustion of a carbon particle.

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So, these are the course contents. There are about 13 topics here. We will first start with fuels; fuels are the basic species which are very important for our course, that is for combustion and their properties.

We have to first know about the different types of fuels and their properties. Then in the second topic we will review the basics of thermodynamics especially with respect to ideal gas and ideal gas mixtures. The third topic will be on stoichiometry. When I say stoichiometry, it means what is the amount of oxidizer required to burn and given amount of fuel? So, that is very important.

After knowing about the fuel, I should know how much oxidizer I should supply. This basically comes after we decide what is the rate at which fuel is fed into a combustion chamber. Once I know that then along with the fuel how much oxidizer, so, normally, say air is the oxidizer which is available in atmosphere it has oxygen and this oxidizer has to be supplied.

So, when you want a combustion to take place, we need two species, one is called fuel species, another one is called oxidizer species. How much amount of fuel is needed is decided by the power rating of the combustor, For example, if I say 1 kilowatt or 1 megawatt etcetera that is the power, which is going to be the thermal power, that is going to be generated out of this combustion chamber; and for that, this much amount of fuel has to be supplied.

So, after deciding that we need to know about how much air has to be supplied to oxidize this fuel. Once the fuel is oxidized then only the thermal energy will be released. The study on how to do the calculations for finding the amount of oxygen required is called stoichiometry. That will be the third topic which we will cover.

When we burn an amount of fuel in a particular condition what will be the amount of heat which is released or what will be the maximum temperature reached in the combustion chamber these are two important aspects what we require. That is actually dealt by first law of thermodynamics. It is called chemical thermodynamics and first law of thermodynamics deals with that.

Then what are the products which are formed? See we know that this is an irreversible reaction. Combustion reactions are irreversible. Fuel species and oxidizer species are going to react and an entirely different set of species called products will be formed. So,

what are all the products which are formed and what will be their typical composition? that will be known by what is called equilibrium.

For that we need second law of thermodynamics. So, the first and second law of thermodynamics will be applied to combustion problems and that will be dealt in topic 4. Now, as I told you already, we have seen many species here; fuel, oxidizer, products, lot of products are there. That means, this study on combustion deals with multi component mixture.

Lot of species are participating as a mixture in this particular study. Hence, we need to know the mass transfer basics. One more thing is that the fuel need not be in gaseous state always; fuel can also be in liquid or solid state.

The rate at which gases are evolved from these liquid and solid phases are very important. It is also very much important to understand how this evaporation or pyrolysis of liquid and solid fuels takes place. For that, mass transfer basics are very much important. So, we will cover up on some aspects of mass transfer basics in this course.

Then, the rate at which a chemical reaction takes place is very important to understand. For example, I want to burn a particular amount of fuel within a particular amount of time. What should be the length of the combustion chamber I require? how fast it burns? that should be decided before dimensioning the combustion chamber. For that purpose, we need to know what will be the typical rates of the chemical reactions. That will be given by, fundamentals of chemical kinetics. So, that is the 6th topic we will see in this course.

Now, if we go for modeling this combustion. It is very important to understand what are the governing equations required for modeling the combustion process. That will be the 7th topic which is called governing equations for reacting flows.

This is quite different from normal fluid mechanics or heat transfer applications because we need lot of other constituting equations and coupling conditions for modeling a reacting flow. So, those aspects will be covered in this particular topic which is called governing equation for reacting flows.

Now, these are the fundamental aspects. Till now we have seen the fundamental aspects. Now, we will go for applications. We will start studying about; what is the flame? what are the modes of combustion? and what are the characteristics of each mode of combustion? and so on.

For example, if there is a combustion which is taking place and there is a flame zone which is formed, when the reactants, when I say reactants, I mean fuel and oxidizer. When the reactants are supplied to the combustion zone and before reaching that zone if they are mixed then this is; obviously, called a premixed mode of combustion.

Now, when they mix only at the flame zone, that is, they are separately fed to the combustion chamber and they mix only at the flame zone, then we get non-premixed mode of combustion. So, these are the two extreme modes of combustion one is called premixed combustion where we premix the reactants fuel and oxidizer and a reaction takes place.

Now, in the other extreme case, the fuel and oxidizer are not going to be mixed at all and they mix only at the flame zone. Now, we can have lot of conditions in between these two extremes. This will generate lot of modes of combustion and the characteristics of each of these modes are studied from topics starting from 8 to 11. Here we will also cover laminar aspect and turbulent aspect of reacting flows and so on.

The general characteristic of combustion flame, detonation, then laminar flame propagation, flammability limits, quenching and ignition, these are all the aspects which we need to understand when we study about these different modes of combustion. The topics 8 and 9 are the topics which cover with premixed modes of combustion.

Then 10 is the topic which actually covers the non-premixed mode of combustion. Then, 11 covers the turbulent combustion modes. Now, 12 and 13 are called heterogeneous combustion topics where you take a liquid fuel droplet and analyze how it evaporates and how it burns.

Now, please see that till this point we are talking only about the gas phase combustion. So, fuel is in gas phase, oxidizer is in gas phase, they mix and they burn and so on.

Different modes we have been able to talk about there, but when you go to the topic 12, we have a liquid fuel and oxidizer is in gas state.

So, now when we want to burn this, the liquid has to be converted into vapor and mixed with the oxidizer which is in gas phase and we have again some different modes of combustion based upon how we mix it.

So, droplet evaporation and combustion will deal with a particular aspect of how a small liquid droplet will evaporate as well as burn. Similarly, for solid fuels, predominantly for solid fuels we can give examples straight away as wood, coal etc. where basically a lot of heterogeneous materials are present.

For example, moisture, liquid moisture will be there, then we have species, gaseous species which are evolved upon heating this, then we have fixed carbon content and minerals which will be inert and so on.

We will focus our attention basically on a carbon particle combustion. Solid particle how it combusts and what are the features how will you understand these combustion modes and so on. So, these are the 13 topics which we will be covering in this course.

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Books



- (1) S. R. Turns, *An Introduction to Combustion Concepts and Applications*, McGraw Hill, 2010 (Text Book)
- (2) F. A. Williams, *Combustion Theory*, ABP
- (3) I. Glassman, *Combustion*, Academic Press
- (4) H. S. Mukunda, *Understanding Combustion*, Universities Press
- (5) K. Kuo, *Principles of Combustion*, John Wiley
- (6) D. P. Mishra, *Fundamentals of Combustion*, PHI books
- (7) V. Raghavan, *Combustion Technology*, ANE publications



So, coming to the reference books and the textbook I will suggest Stephen Turns an Introduction to Combustion Concepts and Applications, McGraw Hill publication as the textbook for this course. This book covers a lot of fundamental concepts and lot of worked examples and exercises are given. Lot of other books have been given here as reference books.

For example, Forman Williams Combustion theory, Irvin Glassman's Combustion, H. S. Mukunda's Understanding Combustion, Kenneth Kuo's Principle of Combustion and D. P. Mishra's Fundamentals of Combustion and Combustion Technology by Raghavan. So, these are the reference books which we can follow and the textbook will be Stephen Turn's An Introduction to Combustion Concepts and Applications.

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Fuels and their properties

Combustion reaction is an **exothermic oxidation** reaction.

The C atom in the fuel is **oxidized** by O_2 to form CO_2 and H_2 is **oxidized** to form H_2O . In this process, a certain amount of **heat is released** to the ambient (**exothermic**). CO_2 and H_2O are called **major products** of combustion.

Combustion reaction predominantly take place in the **gaseous state**, even though **surface reactions** in certain **solid fuels** are known to take place as secondary reactions.

Therefore, fuels in gaseous state readily mix with air and react. However, liquid and solid (**condensed state**) fuels have to be first gasified (**evaporation in liquid fuels** and **pyrolysis in solid fuels**) before they can mix with air.



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Now, before going to fuels and their properties, let us first see some terminologies here first, we will take combustion. So, combustion is a chemical reaction which involves two species one is called fuel species, another one is called oxidizer species.

These are the two important species together they are called reactant species. This reaction is a chemical reaction which is quantified as exothermic and oxidation reaction. First of all, an oxidation process should take place that means an oxidizer is involved and this oxidizer is going to oxidize a fuel species.

This fuel and oxidizer together are called reactant species and it is an oxidation reaction, but while this oxidation reaction occurs it is also called exothermic meaning the heat is released from the combustion chamber to the surroundings. So, combustion reaction is an exothermic oxidation reaction.

Now, what do you understand about the fuels? fuel means in general we can say hydrocarbon species. So, for example, hydrogen is a fuel species hydrogen is a very good fuel, but always hydrogen cannot be used, but typically we get fuels which are called hydrocarbons, because they consist of carbon atoms. I mean general mechanical engineering application-oriented fuels will contain hydrocarbons, that is carbon atoms and hydrogen molecules.

Now, when we oxidize these hydrocarbon fuels, carbon atoms in the fuel is oxidized by the oxygen to form carbon dioxide. Similarly, hydrogen molecule is oxidized to form water vapor. So, now heat is released when these products are formed why because the fuel and oxidizer (the reactant mixture) will have a higher energy level and the products which are formed say CO_2 and H_2O they are having lower energy level. This difference in the energy level is given out as heat.

We will see some examples also later for this. CO_2 and H_2O which are formed they are called major products. So, when I say major products that means, there are several other products which are also going to be formed they can be called minor products, but the major products are these two; carbon dioxide and water vapor.

So, fuel species are predominantly hydrocarbon species which has carbon and hydrogen. See for example, carbon graphite (solid phase) can alone be a fuel. Similarly, hydrogen can alone be a fuel, but in nature we get combination of these say for example, alkenes, methane, ethane; alkenes of all kinds and several type of things we get.

Similarly, if you take a liquid fuel say petrol and diesel, they are mixture of hydrocarbons. Both carbon and hydrogen are available. They will be oxidized with the oxygen and form CO_2 and H_2O . This is the typical reaction which you are going to be seeing later.

As I told you just before predominantly oxygen is available in the atmosphere. So, we will supply air as the oxidizer. In several applications we will supply air as the oxidizer and the oxygen in the air will react with the fuel species.

So, the predominant reactions, chemical reactions, take place in the gaseous state. Fuel, if it is in gaseous state, will mix with the oxygen in the air and we have to supply energy that is called ignition energy. When we supply this energy then it will start the reaction process and form the products as told in the bullet here.

There are other reactions, for example, if you take the liquid fuel it has to vaporize and vapors of liquid should come out and mix with the oxygen in the air and react to only form the products later.

A liquid cannot burn by itself there are special cases. I am telling about the general liquid fuels like gasoline. For example, if you have a liquid gasoline there is no way it is going to vaporize it cannot react at all. Even if you supply cold oxygen inside it bubbles through it is not going to react, unless it forms a vapor cloud and the vapor mixes with the air and gaseous phase reactions are possible then only it can react.

Now, the exception is there in our own application. If you take solid fuel, a heterogeneous fuel, for example, it has some moisture, trapped gases, fixed carbon and some minerals. When you heat up the solid fuel first the moisture is released. Then the volatiles, the trapped gases, are released. The fixed carbon and minerals which are called ash, they remain.

When this particle, the char particle what we call with fixed carbon and ash together they are called char particle. When they become hot enough then the oxygen from the ambient diffuse towards the surface and surface reactions are possible. That is one of the exceptions, this is called surface reactions with respect to solid fuels, that is heterogeneous combustion. So, we have a solid surface on which a gas diffuses and reacts, other than that predominantly all other reactions occur only in the gas phase.

Fuels can be in any state. This means that we can handle any fuel which is in gas phase, liquid phase or solid phase. Fuels in gaseous state readily mix with air and react.

Anyway, they should mix in proper proportions to react. For any proportion it is not allowed. For example, if you have only 1 percent of fuel and 99 percent of air or 99 percent of fuel and 1 percent of air it is not going to react. There is a limit of mixing of these two which will contribute to the burning process. Those things we will cover later.

Fuels which are in gaseous state does not need any other process before it mixes with air and burns. It is already in gaseous state. Predominant reactions are in gaseous state. So, it can very well mix with the air from the ambient and react upon some ignition source.

But on the other hand, if you have liquid fuel or solid fuel, they are called condensed fuels. You see that the liquid fuels have to be converted into a gaseous fuel by vaporizing that. Evaporation of liquid fuel should occur. Similarly, the gaseous fuel trapped inside the solid fuel has to come out and react. For that, you have to heat this. So, an additional process is involved, for liquid to vaporize and for solid to give out the trapped gases inside. This extra heating process is required for the condensed fuels, condensed state fuels. Then only it will evolve required gaseous fuels for gas phase combustion to take place which is the predominant combustion mode.

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Fuel and their properties



Fuels are classified as **fossil fuels** and **synthetic fuels**. Former are formed over several years through geological processes and latter are man-made. Fossil fuels are also processed before they are used.

Examples of fossil fuels are petroleum crude oil, natural gas and coal. Examples of synthetic fuels are biogas, synthetic gas and biodiesel.

For all fuels, one of the important properties is its **calorific value**, also called **heating value**.

It is the amount of **heat released** (in exothermic reaction) when **one kg of the fuel burns completely** with **sufficient amount of air required for its combustion** and the products are cooled to **298 K** (standard reference temperature).



Let us now see the classifications of fuel and go ahead with that. Fuels are classified into two major categories; one is called fossil fuel and another is called synthetic fuel. The

fossil fuels basically are naturally occurring fuels. Fossil fuels are formed over several years under the ground due to several processes occurring there owing to high pressure, and high temperature involved under the ground.

The vegetations and whatever animals and plants which are buried under the ground are transformed over several years due to geological processes and are converted into fuels like crude oil or coal. And now we have to dig up that and take the required fuels. Anyway, we need to process that later, but they are naturally occurring fuels. Nothing a man should do to make a crude oil or a coal. It is naturally available, but we have to spend some energy to take it out. For example, some pre-processing like cleaning and distillation in case of crude oil, cleaning in the case of wood and so on. So that we can use it for applications and power plants and so on.

Fossil fuels have to be processed before they are used, on the other hand, synthetic fuels are manmade, we have to make it. For example, if we want to make biogas, we have to take some animal waste and make a reactor put this animal waste into that do a process and evolve this gas; that means we have to make it ourselves. Those fuels are called synthetic fuels and fossil fuels are naturally occurring fuels.

Examples of fossil fuels are petroleum crude oil, natural gas and coal. Natural gas is also available when you dig out this crude oil and so on. Coal is a solid fuel. So, we get all types of fuels from the ground for example, petroleum crude oil is liquid state fuel, natural gas is a gas, and we have coal which is a solid. So, all the three types of fuels are available from the fossil fuels from the ground.

Synthetic fuels on the other hand we have to make it as I told you. Biogas is the example which involves usage of say animal waste. It is a solid waste or some plant waste. Fermentation is the process done in a particular reactor under particular conditions so that you get biogas. The yield of biogas and the composition of biogas will be dependent upon the source from which it is formed.

Similarly, to produce synthetic gas also called syngas we use the solid materials like coal and biomass and subject to some process like gasification. We have to design the reactor and use these sources there and get the products which are good fuels.

Why we have to generate this because we cannot depend on fossil fuels for long time, just because they are already formed and we are trying to just deplete it. Use it for our purposes and the energy demands are increasing all over the world. We cannot generate that as I told you the fossil fuels are formed over several years. They cannot be formed at the rate which we use.

That means, we should also try to produce our own fuels. Synthetic fuels like biogas, synthetic gas, biodiesel which will substitute some part of fossil fuels. Else we will just deplete the fossil fuels and find nothing later.

So out of these fuels, again you can see that in the synthetic fuels we can generate liquid fuels and gaseous fuels. Normally we do not generate solid fuel from the synthetic processes, we will try to gasify a solid or gasify a liquid to get the gaseous fuel.

Similarly, we can produce solid from liquid or gases from liquid fuels, but solid fuels are not generally formed they are available from renewable sources. For example, sugarcane bagasse, corn starch, rice husk, rice straw, wheat straw and so on. These are actually plant wastes. Similarly, animal wastes like cow dung can be used to produce these fuels. Predominantly we can see that solid fuels and solid wastes are used to produce gaseous fuels as well as liquid fuels.

Vegetable seed is used to extract a vegetable oil and vegetable oil is processed in a process called trans-esterification to get biodiesel. You see that you normally get solid materials from plants and animals and from that we try to process in a suitable reactor to get gaseous fuel or liquid fuels as synthetic fuels.

Now, in many cases we also use the fossil fuel coal, to get the synthetic gas, why because coal burning is not very easy to do. In the recent years we have gone to what is called clean coal technology. We need to understand how it can be converted into some

cleaner fuels as I told you the solid fuels are not very clean; they are heterogeneous in nature.

Because of the mineral content which is called ash and also because of say sulfur and also moisture. In several cases moisture also will be high. So, moisture, sulfur and ash are the things which are making the coal or other solid fuels very heterogeneous in nature and also not very clean.

So, clean coal technology allows us to use some processes in which we convert coal into synthetic gas or some liquid fuels which are much cleaner than coal itself. So, in the manmade fuels we can have lot of choices, but we end up in producing gaseous fuels as well as liquid fuels.

Now, coming to the properties one common property in all the fuel solid, liquid or gaseous fuels is its calorific value or heating value. So, I want to construct the power plant say 2 megawatt in nature. For that I need to burn some fuel to generate thermal power.

Thermal power should be higher than the electrical power, let us say 2.5 or 2.6 megawatts of thermal power produced. Taking into account the conversion efficiency, I will produce around 2 megawatts later.

This thermal power of 2 megawatts is achieved by burning certain amount of fuel. It may be solid, liquid or gaseous fuel. For that, when I burn 1 kg of fuel I should know how much energy which is coming out. That is called calorific value. So, a calorific value is the heat released. Because combustion reactions are exothermic in nature. That is, the heat which is released when 1kg of the fuel completely burns, again there is a efficiency there. See when I say completely it is only my wish, but I do not know whether I can normally burn anything completely, it is not easy to burn everything completely. Especially, when you go for solid fuels, it is not easy to do because there are lot of challenges in burning that because of the heterogeneity of the fuel especially with the ash content and so on.

What we envisage here is when we try to completely burn it, what is the heat released when you burn 1 kg of fuel that is defined as the calorific value. So, now when I design my power plant, I will use the calorific value, but I will also add efficiency there to calculate.

So, when I say if 'x' kg of fuel is required to achieve the power say 2 megawatts, I will say I will use 'x' into 1.1 or 1.2 times that. So, 'x' into 1.2 I will burn so that I will surely reach that power capacity and so on.

When I say calorific value, these are all done in a standard condition. There should be some standards for that. I cannot do, see one can burn in a particular temperature and say this is the value I got. Other can burn in a different condition and report different value. So, there should be some standard to specify the calorific value, what is the standard?

The standard is, when I maintain the temperature of the reactants at 298 Kelvin and burn this in any process and form the products. When the products are formed heat is also released now you try to extract all the heat and cool the products again to the same temperature of 298 Kelvin.

Standard reference temperature is 298 Kelvin (25 degrees), when you cool it to 298 kelvin you will extract the heat from that. So, what is that heat? that heat is called calorific value. 1 kg of fuel should burn for that.

So, calorific value is one of the important (common) properties which we have for all the fuel and we should know that. You can use devices like bomb calorimeter to measure the calorific value of a particular fuel.