Fundamentals of Combustion

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Lecture - 29

Characteristics of Combustion Flame and Detonation – Part 1

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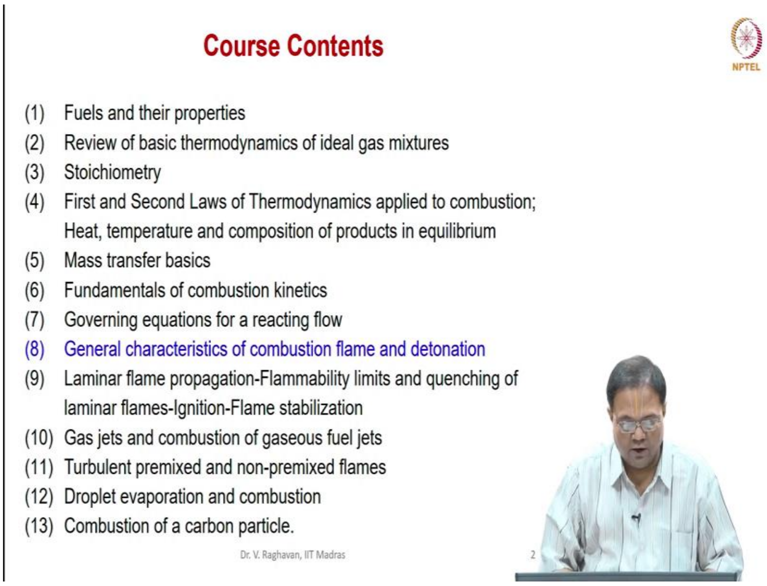

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The next topic is general Characteristics of Combustion Flame and Detonation. We are going to see the characteristics of premixed combustion in this.

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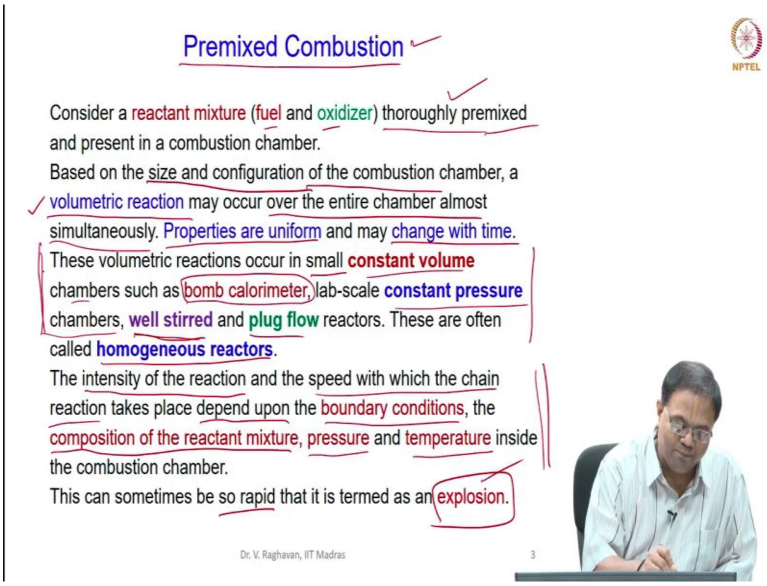

Premixed Combustion

Consider a reactant mixture (fuel and oxidizer) thoroughly premixed and present in a combustion chamber.

Based on the size and configuration of the combustion chamber, a volumetric reaction may occur over the entire chamber almost simultaneously. Properties are uniform and may change with time.

These volumetric reactions occur in small **constant volume** chambers such as bomb calorimeter, lab-scale **constant pressure** chambers, **well stirred** and **plug flow** reactors. These are often called **homogeneous reactors**.

The intensity of the reaction and the speed with which the chain reaction takes place depend upon the boundary conditions, the composition of the reactant mixture, pressure and temperature inside the combustion chamber.

This can sometimes be so rapid that it is termed as an explosion.

So, premixed combustion, consider reactant mixture that is fuel and oxidizer thoroughly premixed and present in a combustion chamber.

When I say thoroughly premixed it should be uniform everywhere. So, within the combustion chamber, when you see the concentration of fuel or oxidizer; it should be uniform everywhere. So, that is meant very thoroughly premixing the reactant.

Now, based on the size and configuration of the combustion chamber, a volumetric reaction may occur. So, volumetric reaction means entire volume will sense that reaction; that means the reaction will occur simultaneously at every point in the reaction chamber.

So, over the entire reaction chamber simultaneously, almost simultaneous, there will be some lag; but that will be very small lag, but the combustion chamber itself is very small. So, from the point of ignition, it actually reacts almost simultaneously everywhere.

So, we call such a reaction as volumetric reaction; over the entire volume that reaction takes place. So, this is possible when the chamber size is small, very small chamber size. So, as I told you, thoroughly premixed reactant; so the properties are expected to be uniform, so uniformly distributed properties, the mass fractions etcetera.

So, temperature, unburnt temperature, initial temperature of the reactants everything will be uniform. Also, once the products are formed; then the product composition also will be uniform and the temperature, the flame temperature will be uniform and this may change with time. So, at every time instant slowly the products may be formed. So, within a short period of time, we can see that the properties can change but it will be uniformly distributed over the entire combustion chamber.

Now, such volumetric reactions can occur as I told in small reactors which may be constant volume chambers, so rigid chamber. Bomb colorimeter is one of the examples. In this bomb colorimeter, we have a constant volume chamber surrounded by water bath.

So, once reaction takes place, the water will receive the heat of the combustion and by noting the temperature rise in the water, we will know what will be heat release. So, by that we will know the calorific value. So, that is the main intent of this bomb calorimeter normally a constant volume chamber.

Then you have a lab scale constant pressure chamber. So, lot of experiments you can do in small constant pressure chambers where the pressure is maintained constant by piston moving in a cylinder. So, constant pressure chambers this will give you lot of characteristics.

So, say for example, if we want to do kinetic steady, we can do with that. Similarly, these are all systems, you do not have mass transfer in this. But we have two more reactors, small reactors called well stirred reactor.

As the name suggests, the reactants flow into this chamber; they are actually very well mixed and they come into the chamber and once they flow through the chamber, the products are formed and the products leave the chamber.

So, it is well stirred; that means that always the quantities will be uniform. So, that is the well stirred reactor. Similarly, plug flow reactor is another type of reactor, where we can make measurements of a species etcetera.

So, these small reactors are used to make kinetic studies. If we want to know the reaction rates of several elementary reactions etcetera, we will use these. So, these are called homogeneous reactors there is no fluid dynamics in this.

So, no diffusion, because always uniform distribution of the species are there. So, there is no concentration gradient. Similarly, the flow is very low; the flow is negligible. Even when there is a well stirred reactor or plug flow reactor, the flow is well resolved in that. So that there is no need to do flow studies thoroughly; like for example, need not solve equations which governs the flow.

So, the main aim of these homogeneous reactor is to study the chemical kinetics alone. So, once you have a well resolved flow and there is no gradient, so that no diffusion etcetera, only kinetic will control the combustion process. So, these reactors are going to be useful in that, so there kinetically controlled reaction process can be studied in this.

So, these are all lab scale reactors, small in size. So, as I told you based on the size and configuration of the combustion chamber, we can get volumetric reaction done over this. So, that is what we are aiming to do in this.

So, instantaneously or simultaneously, the reaction will be complete over the entire volume; we can measure the temperature, pressure, volume everything. So, based upon that, we can fine tune our kinetics.

So, the intensity of the reaction or the speed with which the chain reaction takes place; basically what I am trying to say here is the rate at which the reaction takes place will depend upon several factors. First boundary condition, if you remove the heat very fast; then the reaction will not be very fast.

So, we have to have a good temperature rise for faster reactions to take place. Similarly, composition of the reactants, equivalence ratio etcetera, composition, fuel type itself.

For example, hydrogen air mixture will behave differently than the methane air mixture. Then pressure of course, the pressure will be very important; temperature, you all know the temperature will control the reaction rate very much. So, these are the factors which actually affect the rate or the speed or the intensity of the reaction.

So, in several cases, for example, if you have say hydrogen, oxygen mixture or any fuel with instead of oxygen if you have air, then the air will have nitrogen. So, lot of nitrogen will actually dilute the mixture, instead of that; if you have pure oxygen, then the reaction rates can be so rapid that explosion type of reaction can occur.

That means very rapid reaction, very fast explosion is the process, where there is a very fast completion of reaction. Normally it occurs in a constant volume chambers and the pressure rise will be very high and the chamber itself can explode. So, that is the way the reaction can complete.

So, when there is a premixed combustion, predominantly the chemical kinetics is going to control it. If you can resolve flow, diffusion etcetera to a well known parameter and it is not going to affect the process; then we can say entirely the chemical kinetics is going to take care of this process.

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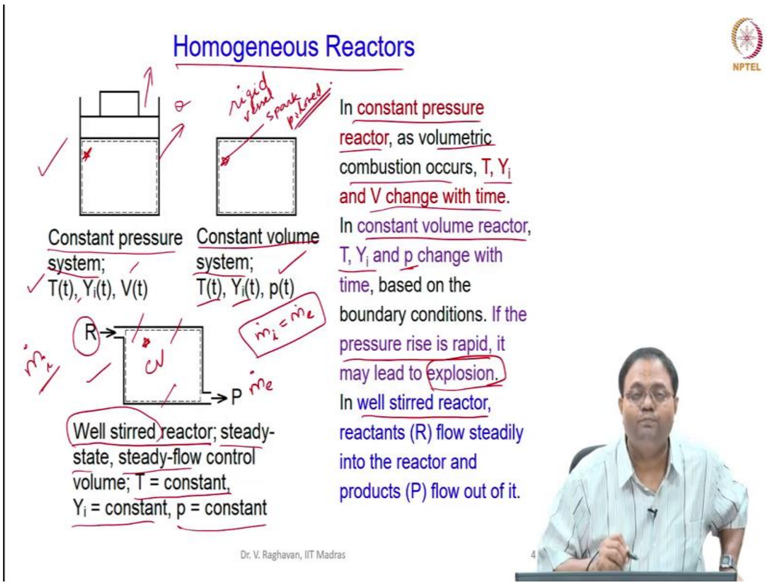

Homogeneous Reactors

Constant pressure system; $T(t), Y_i(t), V(t)$

Constant volume system; $T(t), Y_i(t), p(t)$

Well stirred reactor; steady-state, steady-flow control volume; T = constant, Y_i = constant, p = constant

In constant pressure reactor, as volumetric combustion occurs, T, Y_i and V change with time.

In constant volume reactor, T, Y_i and p change with time, based on the boundary conditions. If the pressure rise is rapid, it may lead to explosion.

In well stirred reactor, reactants (R) flow steadily into the reactor and products (P) flow out of it.

So, let us see some of the chambers like homogeneous reactors.

So, as I told you, we can have a cylinder and piston where the constant pressure can be maintained. When pressure is slightly built up, the piston can move up, so that the pressure inside will be the same.

So, constant pressure system, I say system; that means there is no mass transfer allowed here. We know that as a function of time, as reaction proceeds, T, temperature can vary with time and mass fraction of all the species can vary with time.

Similarly, the volume will increase when the reaction takes place. So, this you can monitor with this; then it is a constant volume system.

So, you can also have boundary condition; see for example, when you have this, we can have Q, some heat can be transferred from this or we can have some other adiabatic boundary condition, we can also say Q equal to zero, So, adiabatic condition and so on.

So, several boundary conditions can be implemented in this. When I say constant volume system, this is the rigid vessel; so these are rigid vessels. So, in this what happens is; as the reaction takes place, pressure actually increases with time. So, this is the pressure vessel, where we will allow some amount of pressure rise; it may withstand, say some 5 bar or 10 bar something like that.

So, some level of pressure rise is allowed in this. So, temperature will vary with time, mass fraction of species will vary with time. So, normally these chambers can be spherical in nature also.

Then as I told you, the well stirred reactor. A well stirred reactor is a steady state steady flow reactor, it is a steady state reactor, we know the amount of reactants coming in. It is the mass flow which is coming in, mass flow rate of the reactant say it is $\dot{m}_i$, it is a inlet mass flow rate and the rate at which the products leave. So, inside combustion completes, products leave at the rate of $\dot{m}_e$ and this is same.

So, both are same here, the mass flow rate of the incoming reactants will be same as the mass flow rate of the outgoing products. So, this is called steady flow and it is in a steady state. Whenever the reactant comes in, it has enough time to burn and the products are formed within this control volume and the products leave.

So, this is well stirred reactor. So, here, there is mixing process which is so good. So, that it is called well stirred. So, that always at any point in time wherever you measure, whichever point you measure, the concentrations will be uniform. Temperature will be the same and so on.

So, that is well stirred condition. So, this you can see that, when you have a type of reactant is fixed; flow rate is fixed etcetera under steady state.

So, initially there will be some transient nature, some time dependent variations will be there but after that quickly it will go to a steady state where temperature will be constant, mass fractions will be constant and the pressure will be constant.

So, in a flow process, normally pressure is expected to be constant. So, these are the reactors which normally we use for validating the chemical kinetics parameters.

So, as I told you in a constant pressure reactor you know that the volumetric combustion occurs and T, Y_i and V change with time, because pressure is constant. So, volume will increase, because of the movement of the piston.

The second is constant volume reactor, volume is constant, so pressure increases when the reaction proceeds, temperature increases and we will know the changes in this. But uniformly distributed content will be there inside the chamber. So, based upon the boundary condition, the pressure rise can be rapid. We call it explosion.

So, normally we will have some pressure relief valve or something like that. So, once the designed pressure or the maximum pressure of the vessel is known, that pressure maybe little less than the pressure that has been attained inside the chamber. Then a relief valve will open and the contents will be allowed to go out. So, this pressure rise can be so rapid that explosion can occur in this.

On the other hand, if you have this well stirred reactor, it is a flow process. So, reactants are flowing at a steady state and as they flow into the control volume; they convert into product and the product flow out in the steady state and this is steadily maintained. So, that you know wherever we measure the temperatures and concentration etcetera will be same.

So, now, by varying the flow rates or varying the reactant types etcetera; we can do several experiments in this. So, these are the reactors which are used for kinetic studies, homogeneous reactors, see there is no identifiable location where reaction is taking place, everywhere reaction will take place. So, it is a volumetric combustion chamber.

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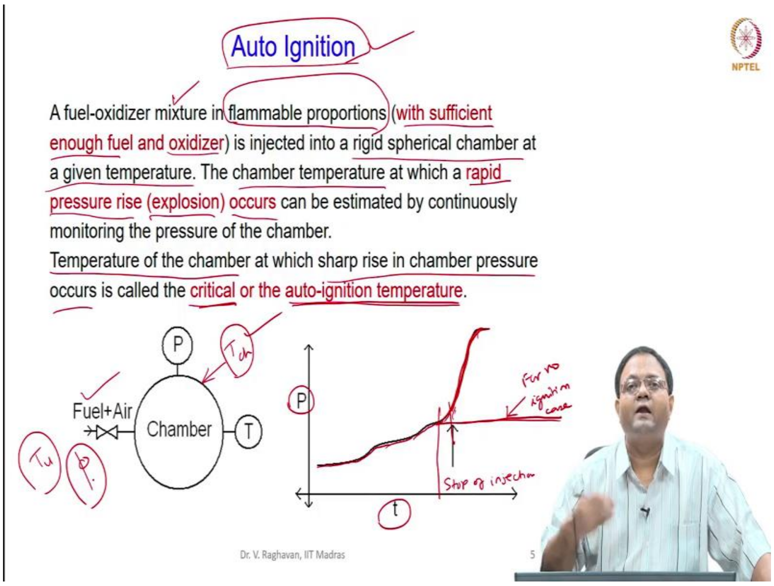

Auto Ignition

A fuel-oxidizer mixture in flammable proportions (with sufficient enough fuel and oxidizer) is injected into a rigid spherical chamber at a given temperature. The chamber temperature at which a rapid pressure rise (explosion) occurs can be estimated by continuously monitoring the pressure of the chamber.

Temperature of the chamber at which sharp rise in chamber pressure occurs is called the critical or the auto-ignition temperature.

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Now, let us see one more thing; see in the in these cases you know, normally we should have some ignition sources. Especially when the reactants are fed at the very low temperature so initially the reactant can be at temperature of 298 K.

So, it means in this well stirred reactor, the reactants can flow in with the temperature of 298 K. But as you basically have higher temperatures, you need not provide ignition; but in the cases of low temperature reactants, the ignition source will be normally provided. Let us say a spark or something should be provided; after this spark is provided, immediately the reaction will take place at all locations, because the chamber itself is smaller.

So, when the reactant comes in; there will be a spark in the well stirred reactor, so that the products are formed and the products move out. So, this is called piloted ignition; when you have an external source, which will supply the energy for taking the reactant to the activated complex, from that the products can be formed.

So, this is called piloted ignition. So, this maybe a spark and this is called piloted ignition. So, this pilot ignition basically is required when the reactants are at low temperature.

On the other hand, we now are going to talk about the auto ignition process. So, in this what we try to do is, a fuel oxidizer mixture this should be in flammable proportions. I will define this more thoroughly later; but what is flammable proportion? This should have sufficient amount of fuel and oxidizer; if fuel is not sufficient, it will not be flammable.

Similarly, if pure fuel is there, say hydrogen is there; but not enough oxygen, then it will not burn. So, when I say flammable proportion; there should be sufficient amount of fuel and oxidizer present in the reactant mixture.

Now, such a reaction reactant mixture is injected into the rigid spherical chamber; rigid, it is a constant volume chamber that is spherical in shape. Now, at a given temperature; whatever be the temperature we can send it? It may be a reference temperature, T = 298 K.

However, the chamber itself can be at a higher temperature; the reactant can enter at a lower temperature, but chamber is actually maintained at a higher temperature. So, I say T chamber ok.

The chamber temperature; we have to maintain this at a particular temperature, which is higher; say for example, 200^{o}C, 500^{o}C something like that. There is a particular chamber temperature at which rapid pressure rise which we call explosion takes place.

So, what happens is, this is the pressure and time diagram. You can see that as the reactants are injected slow pressure rise is happening; reactants are slowly injected, so pressure rise is slow. Then after particular point you can see that, pressure rise is sudden.

So, in this point you can see the pressure rise is very sudden, that is because reaction has now taken place. Now, till this point gradual pressure rise occurs; this is because you are trying to fill the chamber with reactants.

So, the pressure inside there was nothing initially, the reactants are slowly fed. So, in a constant volume chamber; when the reactant enters, slowly the pressure rise takes place.

After particular point, if the chamber temperature is sufficient enough, then automatically ignition takes place and the pressure rises. So, this is called auto ignition.

So, temperature of the chamber at which a sharp rise in chamber pressure occurs, like this sharp rise occurs is called critical or auto ignition temperature of the chamber. So, this is the auto ignition; there is no spark or anything here.

What is happening here is, we are trying to test the mixture, which can be any combination of fuel and air with any equivalence ratio say Φ. This can be injected at the unburnt reactant temperature or reactant temperature and the chamber to which this reactant is fed that is at a particular temperature called chamber temperature which is going to be varied now. So, several experiments can be done.

Now, this chamber temperature will be varied. So, initially it may be 350^{o}C; then you will see that, when you inject at a lower temperature, when the chamber is at lower temperature, no ignition take place. Then the pressure will now be steady like this, it will not vary at all; this is the stop of the injection. So, I stop the injection here.

So, the pressure has raised little. Then there will be no variation in the pressure, if the ignition has not occurred. So, this is for no ignition case; when there is no ignition, the pressure will not change at all. But if the ignition has occurred, then there is a sharp rise which will take place; pressure will be very large, increase very rapidly.

So, that temperature is called critical temperature or the auto ignition temperature. There is no external source of igniter like a spark or a flame, pilot flame etcetera; this is only due to the temperature of the chamber itself. The reactant mixture will attain its auto ignition, that is it will automatically ignite.

So, that feature is called auto ignition. So, for example, when there is a flame and reactants are fed into this. So, the flame itself will sustain by consuming the reactants. So, the sustaining of a flame also will be factor which is governed by auto ignition.

So, this is the experiment, where the chamber pressure can be varied and then for a given reactant mixture and its condition say Φ unburnt temperature etcetera; we will know what will be the auto ignition temperature.

So, when the Φ varies automatically, the auto ignition temperature will vary. For example, for a stoichiometric mixture, auto ignition temperature may be say 500^{o}C; but if you go to lean, you may require higher temperature to ignite and so on.

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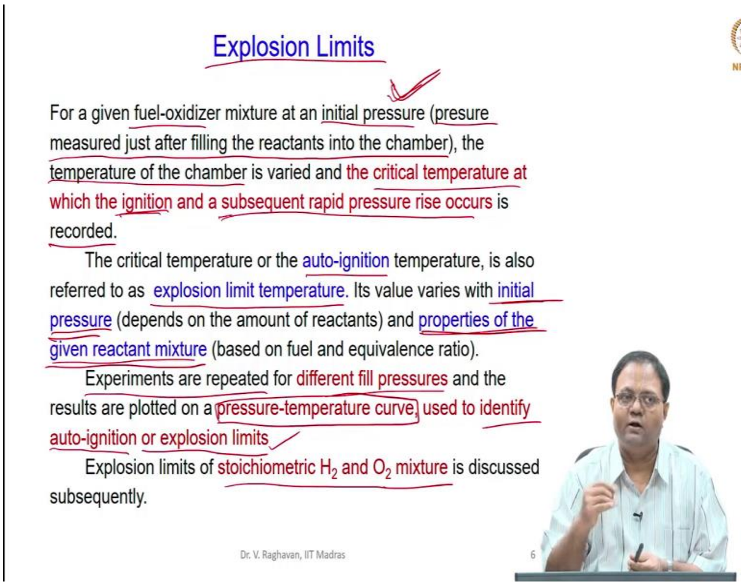

Explosion Limits

For a given fuel-oxidizer mixture at an initial pressure (presure measured just after filling the reactants into the chamber), the temperature of the chamber is varied and the critical temperature at which the ignition and a subsequent rapid pressure rise occurs is recorded.

The critical temperature or the auto-ignition temperature, is also referred to as explosion limit temperature. Its value varies with initial pressure (depends on the amount of reactants) and properties of the given reactant mixture (based on fuel and equivalence ratio).

Experiments are repeated for different fill pressures and the results are plotted on a pressure-temperature curve, used to identify auto-ignition or explosion limits.

Explosion limits of stoichiometric H_2 and O_2 mixture is discussed subsequently.

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Now, so as I told you, this auto ignition temperature leads to a rapid pressure rise, rapid pressure rise and we call it explosion. So, this is also called explosion limit temperature; that is what we are going to see next, explosion limits.

So, this is carefully done for several fuel air mixtures and when we talk about explosion; we will normally use oxygen, instead of air. Now, let us take a given oxidizer fuel combination and it is at an initial pressure. So, this is the initial pressure which is attained just after filling that. So, you are filling it to some volume, so some pressure you are filling it.

When you inject some volume, it will attain a pressure; if you increase the volume, the pressure will be higher. If you decrease the volume, the pressure will be lower. When I say volume, I am saying the volume of the charge which is fed.

The rigid vessel will be constant volume and the charge which is the reactant mixture which is going to be injected into this, will also occupy the entire volume. But the quantity, say the mass, which has been injected into that, that will be varying; if that varies, the initial pressure will vary.

So, if there is an increase in charge, initial pressure will increase and so on. So, this pressure, initial pressure is the pressure which is measured just after filling the reactants into the chamber. Now, as I told you before, the temperature of the chamber is maintained at higher value that is varied now. So, based upon the initial pressure; the temperature of chamber is varied and we record whether the critical temperature is attained or not.

So, what is the temperature of the chamber; that is the critical temperature or auto ignition temperature at which an ignition and subsequent rapid pressure rise occurs, that is recorded for several pressure values. So, I inject the reactants to some level, so that the initial pressure is maintained constant. We know the initial pressure and for that pressure, what should be the chamber pressure?

So, I will vary the chamber pressure. So, now, I will only inject that much quantity and now vary the chamber pressure, such that I will know for the given charge; what is the temperature of the chamber which will ignite. So, chamber temperature is varied actually; so that will cause the ignition and subsequent rapid pressure rise.

So, this is recorded, do you understand. I am repeating the experiments. Now, these auto ignition temperature what I am recording that is also called explosion limit temperature and its value, the explosion limit temperature will vary with initial pressure. That is the amount of reactant and the properties of the given reactant mixture, obviously, because the equivalence ratio, fuel type and so on is varying. So, based upon that, this value will increase or decrease.

So, now I repeat my experiments. As I told you I will first take a mixture that is fixed, say hydrogen, oxygen. Then I will know the composition say, hydrogen, oxygen, let us take stoichiometric proportions. Now, I will now inject say x grams or x milligrams into the chamber. Now, that will lead to a given initial pressure. So, that I know, I record that. Now, I try to vary the chamber temperature, such that auto ignition occurs. So, that will be the explosion limit for me that I will record. Now, I will repeat the experiment to ascertain that there is a value; then I will increase the initial pressure by injecting more charge.

Then what is the value? I will record that slowly. Then finally, I will repeat that for several Φ value, unburnt temperature everything.

So, I can vary the initial pressure as well as the properties of the reactant mixture which is the type of fuel and equivalence ratio, initial temperature of the reactant and so on.

Once I do this experiment thoroughly; what I do is, I repeat the experiments with different fill pressures, that is charge, different charges in the reaction chamber. The results what I obtain for a given mixture, they are plotted in what is called a pressure temperature plot. I will get a pressure versus temperature curve.

So, this is very important to identify the auto ignition limits or what we generally called explosion limits. Why I say explosion? Because this result in a very rapid pressure rise; normally explosion is characterized by such a rapid pressure rise. So, I call this as explosion limits.

So, what I do here, I will repeat; I will first choose a reactant mixture. See for example, we are going to now see the characteristics of stoichiometric H_2 - O_2 mixture; O_2, it is not air O_2, H_2 - O_2 mixture and so I will first fix this.

Now, what I do? I inject certain quantity into the chamber then it will give you us the initial pressure value for that charge, say x milligrams and so on.

Now, I increase or decrease that will result in an increase or decrease in the initial pressure of the chamber with the reactants. Now, the chamber temperature will be varied for this particular initial pressure, so that we will ascertain where the critical temperature, the ignition and pressure rise occurred.

So, if you go to the previous slide, I do not get only a flat pressure variation after the charging is over, then no ignition has taken place. But, if ignition has taken place, I will go to a sharp pressure rise; I will see that and record that.

So, based upon that for every pressure, I will get the temperature at which the ignition occurs. So, such a data is plotted in pressure temperature curve. Now, that will give you the limit. So, let us see the example of stoichiometric, hydrogen - oxygen mixture.