Fundamentals of Combustion Prof. V. Raghavan Department of Mechanical Engineering Indian Institute of Technology, Madras

Lecture - 30

Characteristics of Combustion Flame and Detonation – Part 2

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So, this is pressure; I am taking mm of mercury column and temperature in degree centigrade. So, this is the way the plot looks. Normally what I do as I told you, I increase the pressure slowly from lower pressure and for each I will know what will be the temperature at which the ignition occurs and so on. So, that will result in this curve; it is called say inverted s curve, z curve something like that.

So, in this we see to analyze this curve; we will go through this plot slowly. So, this temperature and pressure corresponds to initial charging condition. As I told you, this will be the pressure of charge. What is the temperature of the chamber at the charging conditions, that is this. So, with that temperature whether there will be an ignition or not that is going to be ascertained.

Now, explosion limits are explained by considering the temperature and pressure dependencies of the elementary reaction. Now, as I told you, it is completely kinetically controlled, there is no big flow or concentration gradient etcetera inside.

So, no diffusion, no transport processes; the only thing which is going to control this is chemical kinetics. So, we need to understand the explosion limits by considering temperature and pressure dependencies of the elementary reactions in the chemical kinetic mechanism.

So, you should have some knowledge of the chemical kinetic mechanism to understand why this happens; or else there is no way to explain this. So, that is what the important concept you should understand here. So, how to go about analyzing it? See the vertical blue line what I have drawn that is corresponding to a temperature of 500° C.

So, if you see this 500° C, when I say explosion, the temperature is in between this point and this point, the vertical line; I have drawn two lines here, when the pressure is in between these two points for the given same temperature 500° C explosion occurs.

However, when the pressure is increased beyond this point until this point, no explosion occurs for the same temperature; so that is the behaviour here. Do you understand? So, what happens is; when the pressure for the given temperature 500° C of the chamber, if the pressure of the reactants, the fill pressure is less than this point, so very low pressures, then no ignition takes place.

Now, I go to this point. So, I go to this point, now what happens? For the same temperature, explosion occurs that is ignition and pressure rise is seen. So, the magnitude of pressure rise can be varying, that is possible, but there is a sharp pressure rise when compared to the full pressure. Next, after this when you increase the pressure further at the same temperature, there is no ignition.

So, you have seen that there is something which we cannot explain unless we go through the chemical kinetic mechanism; that is the important concept here. So, how will you explain this otherwise? With only properties like pressure, temperature, we cannot explain this. Because it is a stoichiometric mixture, Φ is constant. So, $\Phi = 1$ that is not varying in this, temperature is also constant.

So, temperature is fixed in the vertical line 500° C. Then pressure I know, so the pressure is in this range, why ignition should occur and in this and in this range why it should not occur; it cannot be explained unless we seek the help of the elementary reactions and their pressure and temperature dependencies.

So, as I told you from the lowest pressure of 1 mm mercury; up to a small pressure rise 1.5 mm mercury, no explosion occurs. This is the region here, small region here there is no explosion which is going to occur.

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How will you explain this? At very low pressure like this 1 mm to 1.5 mm mercury; free radicals are produced by the reaction. So, H_2 and O_2 are the real reactants, it produces H and it also produces the metastable species $HO₂$. I say this is the metastable species because it is going to be stable under only certain conditions; so, we call metastable species, why I will explain here.

So, the initiation reaction produces radicals, then the chain sequence again produces a branching; so more radicals are produced. Again, you can see that one major species and radicals are produced, so propagation reaction.

So, initiation, then you have a branching and propagation reactions; this produces radicals, free radicals. However, when the pressures are very low, the concentrations are very low; so what happens is the probability of the radicals produced and destroyed near the walls of the vessels is actually higher.

So, what happened? The radicals are lost. So, there is no ignition; radicals are produced, but they are lost, the concentration of the reactants also is very low, that is the reason why there is no explosion occurring at very low pressure value up to 1.5 mm mercury. Now, what happened? The first limit, when I put the first limit, horizontal line here; when the pressure increases beyond 1.5 mm mercury, mixture ignites and explodes.

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So, why? Now, what happens is very simple; at sufficient value of pressure that is this value, a second limit what I have drawn here; chain sequence reaction dominant over the destruction. So, that is what I told that now the concentration of the mixture is higher, more radicals are produced; so, the number of radicals which are sustained when compared to what are lost in the walls, they are higher.

So, the reaction sustains; that is, ignition occurs and we get the limit now. So, in this range it continues when the pressure is increased to about 50 mm; so this is 50 mm log scale. So, 50 mm mercury when it increases to 50 mm mercury column; then this continues.

That means, you always see what will be the pressure in this range, starting from 1.5, slightly more than 1.5 mm mercury to 50 mm mercury column; you see explosion occurring, that is the ignition and the rapid pressure rise occurring. Now, after this point; further increasing the pressure, you go to this no explosion mode, why?

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When pressure is more than 50 mm mercury column, then mixture becomes non explosive. So, reason is competition of H atoms. So, again please understand you have to seek help from the kinetics. Now, it is a very simple system $H_2 + \frac{1}{2}O_2 \rightarrow H_2O$, that is the mechanism here; overall mechanism but it has several reactions.

So, 18 to 20 reactions are required to explain this process; that is the importance of kinetically controlled regime. When nothing else controls the combustion phenomena, only kinetics control we need to go and seek the help of the reaction mechanism with the elementary reaction; several elementary reactions to understand the process.

Now, when pressure is more than 50 mm mercury column; then what happens is the mixture becomes non explosive due to competition of H atom between two reactions; chain branching reaction H + $O_2 \rightarrow O + OH$. So, here you can see that H is required for this reaction to occur and produce more and more radicals.

Then, this is a very branching reaction; that means, it is very rapid. And a low temperature chain reaction which is terminating in nature; $H + O_2$, again H is required for this, plus a third body like combustor walls giving this species $HO₂$ and M

Now, what is the problem? Either, this occurs; HO_2 is produced, then HO_2 can be used to produce some radicals. So, as we see here; HO² also can produce radicals. Now, there are reactions which you can produce $HO₂$ basically. So, here you can see $HO₂$ is produced; so that is sustained here in this range of pressure.

So, if HO_2 is produced that can also sustain know, but why it is not helping the explosion or ignition is; $HO₂$ being a metastable species becomes non reactive in this pressure range, that is reason. So, meta stability; in this pressure range, $HO₂$ is stable and reactive; here non reactive, HO_2 is non reactive; so that is the main reason.

So, if H is used to only produce O and O H; the reaction might have continued, but since there is a competition between H_2 to produce HO_2 also. And HO_2 which is produced, it is not helping the reaction to go through and the mixture is non explosive in this range from this to third limit; so this is the limit; so, that is the reason.

So, we need to understand the HO_2 's contribution here. So, basically HO_2 ; if it is fully stable, then it would have reacted. So, you will get only explosion in this range also, but it is not so; under this pressure condition, it is not going to be reactive. So, we get the non explosive nature of the mixture.

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Now, the third limit is when the pressure is around 3000 milligrams. Now, what happens, HO² what is produced in large quantities which was not useful reaction, this produced no explosion limit. But, what happens when the pressure is increased after 3000 mm mercury; this HO_2 will now react to form hydrogen peroxide; H_2O_2 and this is called H2O² sequence and also you can see the radicals produced here.

This sequence becomes sustainable and so again we get the explosive tendency; that means the mixture will become ignitable and pressure rise will be seen. So, this is very important; so the limits are explained with the help of elementary reactions.

Now, when you see here, when the temperature is below 400° C approximately, there is no explosion irrespective of whatever be the pressure; no explosion takes place because the temperature is not enough. There is the minimum temperature required to trigger the reaction, that is not happening here. So, less than 400° C temperature, no explosion occurs irrespective of the whatever be the pressure.

Similarly, when the temperature, see for example, this is limit; so, this 580°C; when the temperature is more than that value, then even at low pressure you will see the explosion; very small quantity of hydrogen oxygen, but flammable, flammable quantity; it will just ignite and give; the magnitude of pressure rise may be low when the initial pressure itself is low.

But you can see that this temperature will provide explosion at almost all the pressures. Sufficient quantity which is injected inside, then it will surely increase the pressure rapidly due to the occurrence of ignition; auto ignition, so this is very important. So, as I told you for this ignition which is only controlled by chemical kinetics; we need to only consult the mechanism with elementary reactions to understand what is happening. (Refer Slide Time: 12:42)

Now, let us quickly see about the explosion limit of hydrocarbons like methane, ethane, propane; mainly the alkanes which are listed here. One interesting phenomena is see for example, so, this is the curve for methane; that means, that explosion occurs only beyond this temperature.

For example, draw a line here; a vertical line here for example, at this given temperature explosion occurs only in this regime; so, when the pressure is higher than particular point no explosion occurs and here explosion occurs. So, no explosion and in this explosion occurs. So, this is basically a simple curve for methane; so for ethane, you will see some straight portion like this; where the regime is extended slightly.

But, when you when you go to higher order alkanes say propane and further higher order alkanes; we see an interesting phenomena, when the temperature is in this range say 300° C to 400° C; we have a cool flame region. See for example, it should be like this; so it should either go like this like methane or like ethane should go like this flat and go like this.

But you can see a dip here; that means, some flashes of flames one or more reaction zones; in the volume you can see one or more reaction zones which has a faint blue emission. It is not a bright blue, it is a faint blue emission that means, some reaction has occurred in a very low temperature regime of 300° C to 400° C.

And that will cause some flame to propagate that is called cool flames; only for higher hydrocarbons this occurs. So, some interesting behaviour is seen in this.

So, basically why it happened? We have to seek the low temperature reaction. So, why this cool flames are occurring? We have to see what is called low temperature elementary reactions. So, reactions are possible at very low temperatures; in the range of say 300 K - 400 K also; reactions are possible, like the oxidation.

So, actually you know this is actually used in say some engines; an IC engines where if you can restrict the temperature rise and you can combust your fuel at a low temperature range; then the production of emissions like NO_x can be reduced. So, that is the low temperature chemistry or chemical kinetics is sought to do such combustion phenomena in the IC engines.

So, the cool flames are the one which are formed with very low temperatures; low chamber temperatures, we get this; so this is about this. Now, we can see that there is such a phenomena; till now what we have seen is volumetric phenomena, the entire volume will have the reaction simultaneously occurring over that and also the properties will be uniform. It may vary with time, but it will be uniform; so spatial variation will not be much.

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Now, let us go to see what is called premixed flame propagation. Now, we have seen premixed combustion where at every point, combustion occurs in a premixed charge a reactant, but that is not an isolated region, where the combustion is going to occur. So, we are now going into what is called flame. What is flame? So, let us see this. Till now our focus was on smaller chambers where volumetric reactions are possible; homogeneous reactors.

Now, what we are going to see is when the reaction chamber is longer; say long tube or something like that or a larger pressure vessel, spherical pressure vessel say some 10 litres capacity 15 litres capacity etcetera; big vessels, then I cannot ignite all over the space; I will have a spark which is given at say may be in spherical size, I will give a spark at the center. In the long tube, I may ignite at one of the ends.

Now when I do a localized ignition; that is a spark or something, piloted ignition, as I told you it is a piloted ignition; external source, then it will initiate the reaction only in a small region, Volume is very big, so a small spark will initiate reaction only at this point. Then, this reaction zone which is formed that will further move out and consume or it may spread and consume the reactants which is present in the chamber. So, this localized reaction zone which is created by a small spark in a small region that is called flame.

So, candle flames; so candle is the fuel which is available and air is available everywhere, but only at a particular point; it is burning; so that is a flame. So, only a localized combustion zone is identifiable, that we call as a flame. And this flame subsequently propagates through the combustion chamber, consuming the unburned reaction mixture present in this chamber; so that is the flame propagation.

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So, the difference between the previous ones were actually we are talking about the homogeneous reactants; premixed combustion occurring all over the homogeneous reactors like this.

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And we talk about auto ignition where again homogeneous combustion takes place inside the chamber and where only chemical kinetics is going to be very important. Now, what we are seeing is the localized formation of a flame due to a small ignition source, propagating along the chamber dimensions to consume the unburnt reactant mixture. So, that is called premixed flame formation; here also kinetics is very important. So, now, what are the factors which is going to affect that propagation of a flame? It depends on several parameters; so, fuel type, equivalence ratio, temperature of the unburnt mixture, pressure, then wall boundary conditions and so on. So, these are the important parameters which is going to govern this.

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Premixed Flame Propagation

Consider a long duct open at either one or both of its ends, filled with a flammable reactant mixture at a certain temperature. When this mixture is ignited at an open end, a combustion wave, also called a premixed flame, is initiated. Initial piloted ignition depends upon the magnitude of the energy source used as well as the volume of the reactant mixture available. A minimum amount of ignition energy and a critical volume of reactant mixture are required for ignition. These quantities depend on the initial temperature and composition of the reactant mixture. Once ignited at its open end, a flame steadily propagates at a subsonic speed. When temperature and reactant composition are uniform and the flame propagation depends only on chemical kinetics. Dr. V. Raghavan, IIT Madras

So, let us see some cases. Let us first consider a long duct or a tube, open at either one end or both the ends.

So, let us say it is closed at one end and open at other end; I try to fill the reactants slowly and it is filled now; uniformly filled and it is thoroughly premixed reactant mixture which is inside that. Sufficient amount of fuel and oxidizer are there and it is flammable; the unburnt temperature is fixed at a certain value.

So, this is the condition. Now I try to ignite this mixture at the open end, then what happens? A combustion wave or a premixed flame is initiated. So, a flame is formed there; localized, it is not formed all over the tube. Only at the end where you are igniting it, there a small localized flame will form and what happens now? This flame will be formed and it will try to propagate.

Now, how to ignite this? So, the ignition; the piloted ignition that is the ignition done by an external source depends on the magnitude of the energy source. If I give a very weak spark, it may not ignite there will be sufficiently stronger energy I should give to ignite it. So, that is the energy content of the spark or the piloted ignition source should be sufficient enough.

Similarly, the volume of the mixture which is ignited also should not be sufficient low. If low volume is present, then we cannot ignite. So, the concentration of the reactant should be higher enough. So, the volume of the reactant mixture also should be sufficiently available.

So, this is called minimum ignition energy that should be supplied. Similarly, critical volume of reactant mixture. These are the two criteria which should be met to achieve the pilot ignition. We will talk about this little bit later, when you do the ignition in the next chapter basically.

But, you have to keep in mind that pilot ignition whenever you ignite with anything it will not occur; there should be a minimum ignition energy for the ignition source plus there should be sufficient volume for the reactant to burn causing the ignition; so, the flame zone is now formed. So; that means that the flame zone is formed only consuming certain amount of reactants and for achieving that you need certain amount of ignition energy.

So, once this ignition is achieved a flame is formed at open the open end. Now, we are igniting the open end; what happens? The flame steadily propagates at a subsonic speed; slow speed, subsonic speed. When you compare to the speed of sound, it is very low velocity or speed; so, it is going to propagate consuming the mixture.

Now, as I told you the temperature and the reactant composition are constant and nothing is moving inside, within the chamber everything is stationary and thoroughly mixed reactant is present. So, now what will control the propagation? The chemical kinetics, so, chemical kinetics-controlled phenomena will occur.

So, that is what the flame propagation; when you ignite at the open end of the duct, you get a steady propagation at a slow speed, that is what is achieved. And that will consume the reactant and the frame will propagate normally at a very steady state. Now, certain parameters are going to affect; as I told you wall boundary conditions, the dimension of the chamber everything will surely affect. The duct itself will affect the rate at which it goes.

So that means, you know the rate of propagation is not constant; when you fix the fuel and air, it is a fuel say methane and air and the composition say $\Phi = 1$.

When you increase the duct size or decrease the duct size and if you cool it or make it adiabatic etcetera, you will see that the propagation rate will vary. So, that is it; it is not just because of the fuel mixture or its unburnt temperature, it is because of the other conditions, lot of other parameters will affect the propagation rate.

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So, now the flame which steadily propagates at the subsonic speed; that process is called deflagration. Now, what happened? Since, you are igniting at the open end now, the products which are formed, hot products of combustion which are formed that will leave through the open end of the duct.

What happens? The flame propagates through; here this is the sketch, the flame, this is the open end. So, flame propagates through the tube like this consuming the unburnt reactants and the burned gas goes away from the open end out. So, it is a steady propagation; so the speed at which it propagates is called SL.

So, this process is called deflagration and the propagation speed is called laminar flame speed; S_L. When I say speed, here it is only one directional flow; so it is not a velocity, it is a speed; the magnitude is what is important.

So, that is S_L called laminar flame speed; S_L . For most of the hydrocarbon air mixtures, this S_L varies in between 40 to 60 cm/s; that will be the speed at which it moves. But, lot of variation when you try to do the experiment in different condition; even if you change the material of the tube, there will be difference in the S^L value.

So, that means the S_L is not the characteristic of the reactant mixture or the unburnt temperature and so on. It is it is going to be affected by several other characteristics. That is very important characteristic; when you have a premixed flame propagation, the first and important characteristic is the laminar flame speed that we have to understand but it is a characteristic, not a property.

So, now this laminar flame speed, this is the speed at which flame steadily consumes the reactant mixture. Normally, we make it adiabatic; so we will insulate this tube so that adiabatic flame speed only we will try to get basically. Now, the reference frame is attached to the flame itself.

Now, I sit on the flame; I see that reactants are coming to the flame at the same speed of SL. But actually what happens? In the laboratory frame of reference; I see a tube in which the flame is propagating, I can see that the flame is propagating as a function of the distance; it is propagating at a constant speed; almost constant speed SL.

But, if I sit on the flame; then I see the reactants are coming towards the flame at the same speed, normal to that flame; so, reactant can come. So, if this is stationary, then reactants move towards this. That is the frame of reference is shifted to the flame itself.

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So, as I told you several factors affect the flame propagation rate; dimensions, as I told dimension of the duct. Actually, very small dimension may not even allow the propagation. So, there should be some sufficient diameter for the duct.

Similarly, if the shape of the duct also like instead of cross-sectional shape circle, it may be square or rectangle that will also affect the propagation rate. Then the loss of heat and radicals, as we saw in the explosion limits; the radicals are lost in the wall collisions. So, that may affect. That means, the type of wall etcetera will also play a role.

Then, the boundary layer adjacent to the wall, say viscous flow, you know viscous fluid is present. So, as the flame moves, there will be a boundary layer which is formed, that may also affect. The equivalence ratio, initial temperature and pressure of the reactants; so, these are the important parameters which will govern or affect the flame propagation, the rate of flame propagation.

Now, in the previous thing; you can see that the flame instead of being straight like this, you can see that flame is slightly curved. This is because of wall effects; wall effects make the flame to be curved. Now, if the dimension of the duct is below a critical value; as I told you know, the dimensions is very important. We are going to see this in detail later.

When the dimension of the duct is below a critical value; very small diameter you cannot take. What happens in that is, when you have a small diameter the volume of the reactants inside will be low; so the heat release which is going to occur with this low volume of reactants will not be able to compensate for the heat loss which is occurring; so what happens? The flame will not propagate.

The heat released due to combustion within the small volume of the duct cannot compensate for the heat loss through the walls; so flame will not propagate. So, this is very important characteristic; this is actually used for our benefit like we can arrest the flame propagation inside some critical areas where the premixed reactants are available. So, this is very important thing; so, the dimensions are going to affect the flame propagation.

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Now, we have seen deflagration; that is almost steady propagation at very low speed, subsonic speed. Now, what happens; I do the other way, I have the open end and closed end.

I now ignite at the closed end; if one end of the duct is closed and the mixture is ignited at the closed end what happens now? Now, ignite here; flame is formed. The flame consumes, this is unburnt; so unburnt and in this region, burnt gases will be there.

Now, the flame will propagate in this direction, SL, and that will try to consume the unburnt reactant. However, in the previous case; when this was open, the products were able to escape out of that, but now what happens? The product cannot escape; so some type of buildup of products will happen; the product reach higher temperature.

So, what happens is, they will try to accelerate the flame, it is not a piston effect; please understand. What happens is the gases that are burnt, they are hot. So, they are going to expand and while they expand, what happens is the pressure builds up to accommodate and the flame is going to be pushed so it is going to be accelerated.

So, this accelerates the flame under certain conditions; what happens is the velocity, initially it was S_L , now that subsonic laminar thing may become a supersonic; it may also reach supersonic velocities, speeds. So, that supersonic flame propagation is referred to as detonation.

So, closed end, ignition products cannot leave so they are going to expand behind the flame, so that the flame is accelerated. While the flame is accelerated, what happens is it may also reach a velocity which is more than the sonic. So, supersonic velocities and this supersonic propagation is termed as detonation. We will not always see this; it is not easy to establish such as this in all practical situations; it is not possible.

So, just take a tube and close one end and ignite it; you will not see supersonic velocities. Maybe, there will be a transient propagation where you can see the increase in S_L values etcetera, but reaching supersonic condition; it is not easy to achieve. So, some unique applications like pulse detonation engines; we can see that.

It is a special type of engine where some pulses of fuels will be fed and it burns and that the pulse will be huge quantity, huge quantity of fuel will be fed into this and that will accelerate and burn faster and so on. So, lot of research have been done in this, but this is very unique application, special applications. So, where we can see detonations; but normally, it is not possible to really achieve that in lab scale.

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Now, some small characteristics of this we will see through some quantitative values or qualitative differences between these two. So, let us say the unburned gas, when I fix the flame at a particular location, it will see unburnt gas approaching it from one side and the burnt gas leaving from the other side. So, actually burnt gas is formed in this basically. So, for deflagration, what happens? The burnt gas actually moves away from the open end.

For the detonation, that burnt gas is not able to move away from the other side that you have to keep in mind. So, what happens? There are the quantities we will try to do, so here c_1 is the sonic speed; that is velocity of sound.

Now, u_1 is any quantity what I am putting here; when I say suffix is 1, then I refer to this unburnt state and my suffix is 2; that is referred as burnt state. So, when I say u_1/c_1 , that is the Mach number; Mach number at state 1 that should be; so approaching velocity.

So, flame is moving at the subsonic velocity; the approaching velocity when the flame is stationary or I sit on the flame, I see the unburnt mixture coming to me with the subsonic velocity. So, for deflagration you will see that the u_1/c_1 ; Mach number is very low 0.0001 to 0.03. For detonation, since the flame itself can move with supersonic velocity, when you sit on the flame you will see the unburnt reactant mixture approaching you at very high Mach numbers.

Actually, it is not easy to achieve this basically. So, in a normal shock you know; normally, it can propagate at such Mach numbers when there is a detonation wave which is propagating; there will be normal shock also associated with that, it is highly irreversible.

So, that 5 to 10 is the range of; so what I am trying to put here is let us say qualitative assessment. Much larger Mach numbers are seen in the detonation. Similarly, what is the ratio of the velocity at that station 2 by station 1? For deflagration; that is the hot gas are going to move away from the flame, out of the duct to the open end they accelerate because of the higher temperature and higher pressure.

So, the ratio u₂/u₁; u₁ is actually very low. So, u₂ we can see the Mach number here; u₂/u₁ is 4 to 6, acceleration will take place. But here deceleration takes place because when compared to incoming or approaching unburnt velocity, detonation velocity, this will be very low. Now, p_2/p_1 ; it is almost constant, when you say slight expansion; it is almost constant, there is no pressure rise at all. But here a strong compression takes place 13 to 55; very sharp rise in the pressure.

Similarly, temperature, some heat addition happens in both; so, there is an increase in temperature 4 to 16 here; here 8 to 21. But larger, at least 2 times larger than the detonation. Density ρ_2/ρ_1 is 0.06 to 25; here it is 1.7 to 2.6; there is some qualitative comparison between a detonation and this. But please understand, this is for a particular condition. So, basically this deflagration is measured for CH₄-air; $\Phi = 1$. So, these are the typical quantities for this particular case some calculation based on normal charge propagation and other with the heat edition and so on.