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

Lecture - 37

Laminar Premixed Flames - Part 5 Ignition of premixed mixture (Semenov's Analysis)

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Started with the premixed flame analysis and discussed about the solution, simplified methodology, what was recommended by Professor Spalding and by solving the energy equation, integrating it twice $-\infty$ to $+\infty$ and $-\infty$ to $\delta/2$, we are able to get some expressions for the laminar flame speed and the flame thickness.

$$S_L = \left[-2\alpha \frac{(1+s)\overline{\omega}_F^{\prime\prime\prime}}{\rho_u} \right]^{0.5}$$
$$\delta = \left[\frac{-2\rho_u \alpha}{(1+s)\overline{\omega}_F^{\prime\prime\prime}} \right]^{0.5} \text{ or } \delta = \frac{2\alpha}{S_L}$$

So, we can see that the laminar flame speed S_L is dependent on the thermal diffusivity α and the average reaction rate. So, this is actually the fuel consumption rate. So, negative term appears here.

So, if you see this S_L , we have already seen from the thermal theory that S_L was proportional to $(\alpha\omega)^{0.5}$. So, same thing is appearing here $S_L \alpha \sqrt{\alpha \overline{\varpi}_F^{\prime\prime\prime}}$, that is the reaction rate.

Then if we take the flame thickness, flame thickness is inversely proportional to the S_L . So, if the flame speed is very high, then the reaction will be completed within a very small regime, so that small regime that is called flame thickness. So, flame thickness we have already seen that it will be of order of millimetres. So, this is the simplified theory based expression what we got for S_L and δ .

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Now, in the comprehensive theory - the third one, we take into account both the heat transfer plus the radical transfer from the reaction zone etcetera to the premixed zone, and it also solves these equations numerically.

For example: whatever one-dimensional equations what we have presented that for all the species, we normally use detailed mechanism for these elementary reactions.

So, when you do that and solve several equations, for example, if there are n species if you solve n-1 equations, energy equation, etcetera, then we will be able to get the structure of the flame in a more detailed manner.

For example, in this case, we have solved for propane flame, premixed propane air flame taking 1 atmospheric pressure and the unburned gas temperature is 298 K.

Under these conditions the flame structure, one-dimensional flame structure has been numerically predicted; by solving set of equations, energy equation and species conservation equations using the kinetic mechanism having 57 species and 536 elementary reactions. It is called comprehensive reaction mechanism; it has been used and this has been solved.

Now, if you see the profiles of say here in this case in the profiles of temperature, we can see the temperature increasing very sharply and reaching almost the flame temperature. This is adiabatic case again. So, adiabatic premixed propane air flame is considered here. So, this is the structure what we got.

And if you see the heat release, the axis in the right hand side, the heat release is very low and sharply increases to a maximum value in the reaction zone. Now, if you see the reaction zone is pretty much say about 1 millimetre, so that is the reaction zone thickness as I told you.

And if you see the right hand side graphs, you will see the propane, the propane is steadily coming in and it is consumed rapidly in the reaction zone, where you can see some CO is produced and it is consumed.

Similarly, oxygen which is coming in, oxygen will be much higher than the propane's mole fraction, again which is coming, and it is consumed in the reaction zone. Products are formed in the reaction zone. You can see the increase in the CO_2 concentration here, similarly water vapour increases.

So, this type of detailed things only we have shown here only the major species like CO_2 , H_2O , the fuel oxygen etcetera. We can also see this reaction mechanism with 536 elementary reactions has several radicals.

So, we can also show profiles of OH, H and other radicals like H_2O_2 , HO_2 , meta stable species etcetera. So much detailed computation can be done by numerically solving the set of equations what we try to solve in a simplified manner taking only one reaction mechanism, one step reaction mechanism into account.

Now, this is very important to understand the structure, accurate flame temperatures then the flame thickness etcetera can be got from this particular analysis. So, here also this is actually a one-dimensional thing.

We can use the software like Chemkin or Flame Master etcetera to get this type of onedimensional flat flame, actually we are trying to simulate a flat flame, and it can also predict the laminar flame speed from this.

So, these types of important things which actually can be carried out, analysis can be carried out for determining the sensitivity of the chemical kinetic mechanism. So, say this species, whether you want any other pathway to represent accurately these etcetera.

So, some measurements can be taken. So, after the measurements are taken, this analysis can be used to validate that and fine tune your chemical kinetics. So, in this way the structure of the flame can be more accurately predicted.

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()Ignition of Premixed Mixture As discussed in $H_2 - O_2$ system, there is a certain temperature, called auto-ignition temperature, at which the reactants ignite and combustion proceeds to completion. Auto-ignition is seen in Diesel engines, where, when diesel is injected into the hot air, it vaporizes, mixes with air and the mixture ignites. There is no external source of energy, such as pilot flame or spark, which is necessary to cause the ignition. When the mixture attains the auto-ignition temperature, the mixture is ignited. On the other hand, in conventional Petrol/gasoline engines, a spark is used to ignite the premixed charge of petrol and air. In fact, it is desired that the charge should not auto-ignite. This method of using an external source to accomplish ignition is called piloted ignition. Dr. V. Raghavan, IIT Madras

Now, we go to the next topic which is the ignition of premixed mixture. So, previously in the previous lecture, we saw about the auto ignition or the explosion limit temperature of H_2O_2 system.

Based upon the initial pressure of the charge and the temperature of the chamber, we determined whether ignition will take place or not, and the reaction will proceed to explosion or not. So, such a scenario where without any additional or external ignition source ignition is accomplished, then such a process is called auto ignition.

So, if you take diesel engines, for example, in diesel engines the air is compressed, air is taken in first and it is compressed and a high pressure and high temperature air will be present in the cylinder.

When diesel is injected as fine droplets into this chamber, it vaporizes almost instantaneously and mixes with the air; and the mixtures auto ignition temperature is already achieved in the chamber, so the mixture will be ignited.

So, such a process is called auto ignition. So, there is no external source of energy like a spark or a pilot flame etcetera provided to cause the ignition, so that is the auto ignition thing.

So, we have already seen for isothermally maintained chamber when the charge of H_2 and O_2 was injected, based upon the pressure at a particular temperature you will get the ignition. So, critical temperature at which ignition is got is termed as auto ignition temperature. So, there is no external source of igniters used in such a analysis.

Now, on the other hand, if you have petrol engine, you know that petrol is a highly volatile matter, so petrol is actually taken into carburettor and in a conventional engine there are lot of improvements done in this sector.

So, if we take conventional engine where carburettors were used, you can see that petrol was taken in with some proportion of air by volume, and this mixture is injected into the chamber and it is compressed. But it will not ignite due to the temperature prevailing there, so an external spark will now work on this.

The spark would give this energy to ignite this charge. The premixed petrol and air charge, it is called premixed charge of petrol and air, so that will be ignited by using an external source of energy provided by a spark which is lying within the cylinder.

So, now basically this will ignite and the flame which is formed near the spark will propagate through the mixture very fast and the complete combustion will take place.

However, please understand that in this petrol engine, we do not require auto ignition that is the main criteria. The mixture should not auto ignite, that is called as knocking. So, if you auto ignite, then it will unnecessarily produce some pressure oscillations etcetera, so that is called knocking and we should avoid that.

Similarly, in several cases, we use what is called external ignition source to ignite the mixture which is coming in, so that is called piloted ignition. So, there are two types of ignition which can be done on a premixed charge.

If you have a hot environment, and the premixed mixture is coming in, the temperature prevailing there itself will auto ignite, so that is one mode, we do not require an additional ignition source there. But in some cases, we need additional piloted ignition sources like spark plug, pilot flames and so on.

So, we will see the characteristics of two types of ignition; now one is the auto ignition, another one is the piloted ignition which is due to the use of external ignition source. (Refer Slide Time: 10:44)

()Semenov's Analysis Auto Ignition Consider homogeneously mixed reactants. Let an amount of reactant mixture undergo auto-ignition and produce products. The reaction rate of a global reaction, Reactant → Product, is written as $M_{P}[R]Aext$ Here, M_R is molecular weight of the reactant and [R] is its concentration. A and Ea are pre-exponential factor and activation energy, respectively. During the ignition, only a small quantity of reactant is consumed. Thus, the concentration is almost equal to its initial concentration. Reaction rate is written in terms of density as, $\dot{\omega}_{R}^{\prime\prime\prime} = -\rho A \exp\left[-\frac{E_{a}}{R_{u}T}\right] \frac{\mu_{a}}{r_{a}^{3}} b$ Dr. V. Raghavan, IIT Madras

Now, let us analyze the auto ignition. Semenov was the person who gave analysis of this. Several people have done, and this is a very famous analysis provided by Semenov.

So, we consider a homogeneously mixed reactants that is uniformly mixed everywhere, the concentrations are the same and the unburnt reactant temperature is the same. Under that condition, we call the charge or the mixture as homogeneous mixture.

Now, some amount of the reactant mixture is going to undergo auto ignition and produce the products. Now, the reaction rate, let us consider the global reaction rate. Please understand that it is a transient process.

So anyway, to exactly find the ignition delays etcetera, we need to employ detailed kinetic mechanism or at least some mechanism which has more species. But in the simplified analysis, normally when we go for theoretic analysis, we simplify the analysis. So now, we have only considered here single step reaction giving products.

So, the reaction rate of such a reaction that is the rate at which reactant is consumed is got by the molecular weight of the reactant M_R into the concentration of the reactants. So, for example, this is kg/kmol into this is concentration is kmol/m³.

$$\dot{\omega}_{R}^{\prime\prime\prime} = -M_{R}[R]A\exp\left[-\frac{E_{a}}{R_{u}T}\right]$$

So, this will give you maybe for this the unit can be 1/s. So that you get the unit of this reaction rate as kg/m³s. So, that is the unit of the reaction rate, kg/s per unit volume.

So, molecular weight of the reactant mixture is M_R , then the square bracket or within the square bracket is the concentration of the reactant. And we know that this is the kinetic parameters, A is called pre-exponential factor, and E_a is the activation energy. So, we know this.

$$\dot{\omega}_{R}^{\prime\prime\prime} = -\rho A \exp\left[-\frac{E_{a}}{R_{u}T}\right]$$

So, for single step reaction we write the reaction rate like this. Now, during the ignition, you can see that the ignition is only a very short period process, a small amount of reactants is consumed and a very small flame is formed.

When, it is auto ignited or anything, a small region is ignited. So, we consider only this space a very small space which is ignited, and now that will produce heat to heat up the incoming reactants.

So, we can take any scenario like that. Only a small quantity of reactant is consumed, therefore, what we assume or what Semenov's assumption was the concentration is almost equal to the initial concentration that is it. So, there is no change in the concentration with time. Ignition itself is a very short period process and within that time the concentration measured will not change much, only a small amount of reactant is consumed. With that we can also write, you can see that molecular weight of the reactant in this concentration is nothing but kg/m³ which is nothing but the density.

So, we can write the reaction rate in terms of density also that is $\rho Aexp(-E_a/R_uT)$. Now, this is again the way to write the reaction rate in kg/m³s. So, this is the first term what we have, which we need to analyze.

Then when you multiply this reaction rate with the heat release that is the heat of combustion, for example, then that will be the heat released in the combustion process. So, this times the Δh_c that will give you the heat released per unit volume. But now, this heat can be lost to the environment.

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So, what is the heat which is lost? Heat lost to the surroundings, let us consider convection as the predominant mode here. We can write the heat loss to the environment as the product of the heat transfer coefficient h which is having a units of W/m^2K and S is the surface area through which this convection heat transfer is occurring and T is the temperature of the homogeneous mixture, and T_w is the wall temperature where the heat is lost. S is the surface area of that wall where the heat is lost.

$$Q_L = hS(T - T_w)$$

So, you can see this is W/m^2K , and this is m^2 , and this is K. So, you get Q_L in Watts. The heat lost to the surroundings by convection is $hS\Delta T$ units is in Watts.

So, now the heat lost is calculated with spatially homogeneous temperature T, the spatially homogeneous temperature is T, whatever area we consider, volume we consider.

Now, the governing equation for the temperature rise of the mixture, see when ignition has to happen the temperature from the initial value of the mixture should increase to the ignition temperature, auto ignition temperature at which the ignition will occur.

So, the rate of change of temperature rise within the volume is nothing but $\rho \times V$ that is the mass $\times c_p$ - specific heat $\times dT$ (temperature)/dt (time), this is the rate at which in the given volume the reactants temperature increases from the initial temperature to the auto ignition temperature, so that is governed by the production of energy which is due to the reaction.

$$\rho V c_p dT/dt = production of energy (Q_R) - heat loss (Q_L)$$

So, we saw in the previous slide $\dot{\omega}_R^{\prime\prime\prime} \times \Delta h_c$, so that will be the rate at which the heat is generated minus the heat which is lost. So, you can see that if this has to increase, the right hand side has to be positive.

This d temperature by d time should be positive. If this has to be positive, then the production of energy should be higher than the heat lost, at least slightly higher than the heat lost.

So, here as I told you V is the volume, ρ is the density, c_p is the specific heat at constant pressure, and this Q_R production term is written as the product of reaction rate kg/m³s multiplied by the standard heat of combustion that is Δh_c that is J/kg and multiplied by volume also to get in Watts. See please understand that the heat lost term is in Watts.

So, if you write the production term Q_R as the rate of reaction into Δh_c , so this will be kg/m³s, and this will be J/kg into volume that is m³. So, now you can see that this will be J/s that is Watts, so that will be the production term.

So, here if you see this term - the left hand side term, this is $(kg/m^3) \times m^3$ is the volume, c_p as J/kg-K and dT/dt that is K/s. So, now if you see this, this will be J/s again Watt; so, the units are consistent between left hand and right hand side.

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So, substituting this, we get the governing equation written as

$$\rho V c_p \frac{dT}{dt} = -\rho A \exp\left[-\frac{E_a}{R_u T}\right] \Delta h_c V - hS(T - T_w)$$

Why minus, because reactants are consumed, so that is negative. For making it positive, we put a negative sign here.

So, $\rho Aexp(-E_a/R_uT)\Delta h_cV$ - heat which is lost which is $hS(T - T_w)$. So, this heat it is we have to subtract that.

Now, this energy, so this is positive. Please understand that since this term is negative basically so we have to put a negative term. We are putting here to make this positive. And the energy release is exponential in nature, this is because of the exponent term, this is exponential in nature.

So, if you plot Q_R as a function of T, the red colour curve shows the exponential nature of increase of Q_R with temperature. The heat lost term is linear that is the blue line show that, so when you vary h as h_1 , h_2 and h_3 .

Then you can get the lines h_1 , h_2 , h_3 , these lines correspond to Q_L 's, Q_{L1} , this will be Q_{L2} , and this will be Q_{L3} corresponding to the values of h_1 , h_2 and h_3 respectively. So, this is the curve you get.

So, let us fix the heat of combustion and the reaction rate. So, Q_R curve is fixed now. Now, based upon the heat loss, ignition will occur. We can also do other way. We can also fix the heat loss and vary the Q_R basically to see where ignition occurs.

So, let us do the other way. Both are same. So, the Q_R is now fixed as one curve. Now, try to vary h, so that you get heat loss lines h_1 , h_2 , h_3 corresponding to Q_{L1} , Q_{L2} , Q_{L3} , and see where ignition occurs and where not.

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Now, same curve is replicated here. Let us take the case of h equal to h_3 this case that is Q_{L3} is the heat loss that is $Q_{L3} = h_3S(T - T_w)$. So, now if you see that the Q_R line is always above this Q_{L3} line, so ignition always occurs.

So, if the heat loss is less, you get positive dT/dt, so that will cause the increase in temperature from the initial value to the auto ignition. Once auto ignition temperature attains, the ignition takes place.

Now, we come to the second case $h = h_2$, there Q_{L2} is the heat loss. Now, you can see that in this case this line touches this curve at a critical temperature say this is critical temperature T_c .

So, when you have this Q_R curve is same, Q_{L2} curve corresponding to $h = h_2$, you can see that this line forms a tangent to this curve at the point c what we call critical point. And the critical point again you can see that. So, other than that point everywhere Q_{L2} is lesser than this. So, ignition will occur.

But the critical point you can see that that values of Q_R and Q_L are the same because the h_2 line the Q_{L2} line touches that Q_R line there. Similarly, the slope at that point that is the mean of tangent for both the curves and line should be the same that is $dQ_R/dT = dQ_L/dT$, so that will be the slopes.

Slopes and the value should match at that critical point. So, now T_c will be the ignition temperature, so that is the way we determine. So, where the heat loss just balances the heat produced, there the ignition will occur, so that is the criteria.

Now, this is fine. Let us try to increase the heat loss further by increasing the heat transfer coefficient to h_1 , now corresponding heat loss line is Q_{L1} . So, where you see that when $h = h_1$, the h_1 line or the Q_{L1} line produces two points by intersecting the Q_R curve at a and b.

And these two points are stationary points, because at that points the values of Q_R and Q_L are the same, Q_{L1} and Q_R are the same, but please understand the slope cannot be same here.

So, now let us understand what are the stationary points here. So, let us take when T less than T_a , $T < T_a$, now this is the T_a and this is T_b

So, now when $T < T_a$, what happens? $Q_R > Q_L$. As per this curve the Q_R is here and Q_L is here, so $Q_R > Q_L$.

So, what happens now? T will increase now to T_a . See, when we are in some point here the q, T will increase because the loss is lesser than the production, so it will slowly increase.

But ignition may not occur, the temperature itself is very low. You can see the heat release is very low, temperature is very low, it may increase the system temperature; however, it may not cause ignition correct.

So, ignition will not occur at that point a, temperature itself is very low. It may not be equal to auto ignition; obviously, it is less than the auto ignition temperature. So, ignition will not occur. Now what happens, the temperature increases and reaches T_a .

So, when the system is less than T_a , and when you talk about h_1 curve, Q_{L1} curve, you will see that $Q_R > Q_L$ and slowly the temperature from the initial value will increase towards the T_a value. And after it reaches the T_a value, then further increase will not occur because now what happens $Q_R < Q_{L1}$.

Now, what happens if $T_a < T < T_b$, so T_a is in between these two anywhere here in between T_a and T_b , then what happens?

The system at these points, we can see that Q_R is always less than Q_L between a and b; $Q_{L1} > Q_R$ value. So, what happens here? The dT/dt will be negative. So, at a temperature between T_a and T_b , the system cools down to a, so that is what will happen.

So, now, please understand in that case when you have a stationary point and you perturb the temperature above or below this stationary point. So, T_a slightly more than T_a or less than T_a , you can see that the system will reach the T_a value.

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So, we call this point a stationary point, as a stable point, where whatever happened the system will come back to the initial state. See, wherever the temperature is greater than T_a or less than T_a , but it should not be greater than T_b that is the only criteria. If that is the case $T_a < T < T_b$, then you can see that the temperature will reach T_a value.

Now, same curve $h = h_1$ only, so Q_{L1} is the heat loss line. And now we consider a situation where $T > T_b$. Now, when $T > T_b$, you can see that $Q_R > Q_{L1}$ is low. So, Q_R is greater than Q_L .

So, system temperature, the right hand side is positive, dT/dt will be positive. So, the temperature increases and ignition occurs, so that is the criteria here. Ignition occurs, obviously, ignition occurs because the temperature is also very high here.

So, it will actually go to explosive limit. Temperature rise will occur. What happens? The system ignites.

So, when you are around this point basically say take point b slightly increase, it any a slight increase in temperature from the point b, with a slight increase in temperature, system immediately ignites. And it goes to a explosive state because the temperature is very high here at this point, temperature is higher here. So, it will go to very rapid rate or to explosion.

Now, from the point b here, when you decrease the temperature slightly, then it is not going to reach b that is what the point is here. When you decrease this, then further cooling will take place. So, system will cool down to point a, it will not reach point b.

So, it is unstable point. So, when you perturb it to the higher value, it will go away from that. So, temperature further increases because of the ignition and explosive nature of the reactions which are taking place, temperature will further increase from this point T_b .

So, please understand that this T_a , T_b , T_c are very close to each other basically, so very close to ignition temperature. So, immediately ignition occurs. But after ignition has occurred, the system temperature will increase rapidly. So, the temperature moves away from T_b , increases from T_b , when you slightly increase the temperature from T_b .

On the other hand when you slightly decrease the temperature from T_b , where the temperature is T_b , when you slightly decrease, then it cools down to T_a , that means, it will never go to T_b at all. So, that is, this stationary point, point b, is unstable stationary point, it is not stable.

Because any perturbation from that point will lead to either rapid increase in temperature from that slight increase will result in rapid increase, or slight decrease will result in rapid decrease to T_a value. So, these are the main things.

So, based upon the value of say the h's - the heat transfer coefficient you get different heat loss lines and based upon the lines we will get different ignition criteria. So, the main ignition criteria is the point c where you should at least have a balance of Q_R and Q_L , so that is what we are going to analyse next.

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At the critical point c, point c is a critical point because there the heat loss matches or the heat loss line forms a tangent to the heat production curve. So, both the value $Q_R = Q_L$ and the slopes $dQ_R/dT = dQ_L/dT$. So, these two equations are valid. So, mathematically if you write this what is Q_R ? $\dot{\omega}_F'' \Delta h_{cv}$. What is Q_L ? $hS(T_c - T_w)$ just balance it.

Now, this is the $Q_R = Q_L$ equation. So, now, this will be $dQ_R/dT = dQ_L/dT$ expression. So, just differentiate this and write this.

So, $\rho Aexp(-E_a/R_uT_c)$. Please understand that I am applying the temperature as T_c here, here also it is T_c , here also right hand side you can see T_c will be appearing. So, now, $\Delta h_c V$ into this product will come here.

So, you apply the product rule for the differentiation. So, Ap^n will be np^{n-1} , so that is what you have to insert here. So, that $E_a/R_uT_c^2$ will come out and that will be right hand side this T_c and T_w , so that will be when you differentiate it, it will be only in hS.

So, you have two equations now. Now, using these two equations, that is you can divide this by this, and get this equation that is T_c , so you are dividing the first equation by the second equation.

So, T_c , $T - T_w$ all other terms cancels $1/E_a/RT_c^2$ will be there that is RT_c^2/E_a that is left hand side equal to $T_c - T_w$ this is the quadratic equation.

So, this has two roots. This is the quadratic equation which has two roots. And the lower one will apply for ignition. The lower temperature T_c , where the lower temperature of this quadratic equation will be the ignition, auto ignition temperature.

So, anyway it is the proper choice of this E_a value, A value, etcetera is required for causing this. So, normally we cannot get accurate value of auto ignition temperature unless we go for some detailed mechanism.

We cannot just use one step mechanism and do it, but this is the concept behind that. So, this is the way we have to do this. So, heat which is generated should at least match the heat loss to cause ignition. If it is less than that, it will not, it will cool down the system. So, this is the analysis of auto ignition by Semenov.

So, we can see that we have we analyzed taking the heat produced to be constant and considering different scenarios for heat loss. And we have argued at what scenario the ignition will take place that is what scenario there will be increase in the temperature of the system from the initial value to the auto ignition temperature. So, that is what we have seen here.