Fundamentals of Combustion

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Lecture - 35

Laminar Premixed Flames - Part 3

Flammability limits and Premixed flame theory

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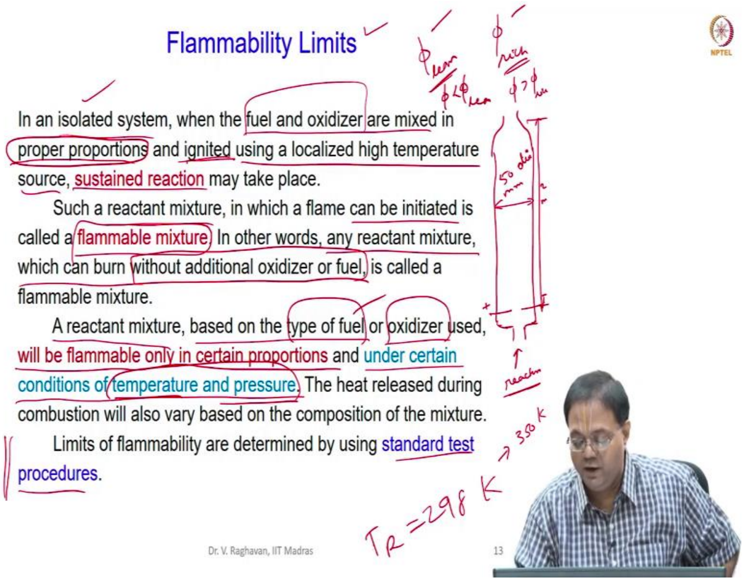

Flammability Limits

In an isolated system, when the fuel and oxidizer are mixed in proper proportions and ignited using a localized high temperature source, sustained reaction may take place.

Such a reactant mixture, in which a flame can be initiated is called a flammable mixture. In other words, any reactant mixture, which can burn without additional oxidizer or fuel, is called a flammable mixture.

A reactant mixture, based on the type of fuel or oxidizer used, will be flammable only in certain proportions and under certain conditions of temperature and pressure. The heat released during combustion will also vary based on the composition of the mixture.

Limits of flammability are determined by using standard test procedures.

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Next topic is the Flammability limits. This is very important to understand. So, if you have a system and I do not allow any mass transfer or heat transfer.

So, it is isolated. So, we have fuel and oxidizer properly mixed and kept in the system. Now, if the fuel and oxidizer are mixed in proper proportions and ignited; ignited means you have to add some heat to that.

So, we just have hydrogen and oxygen in a room, it does not burn, there should be some spark or something, we should ignite it. So, higher temperature source is required to ignite that; room temperature cannot ignite that. Using a localized higher temperature, that is the ignition source, it is ignited. Then what happen? A sustained reaction will take place; so, may be the flame will be formed and it may propagate through the mixture and so on.

Now, such a reactant mixture in which the flame can be initiated using a spark or igniter is called a flammable mixture. So, if you have a mixture which is not able to be ignited.

See even you may have a mixture and you have a spark which is continuously operated on the mixture, it may not be ignited. Only under certain proportions of the mixture, it will ignite. So, they are called proper proportions.

So, any reactant mixture which can burn without additional oxidizer or additional fuel, see I have a lean mixture; more oxidizer is there. Try to add more oxygen to that, it may not ignite after particular point. So that means that it may need some more fuel to burn. Similarly, if you take the mixture which is rich in nature try to add more fuel to that, it may not burn because it may need more oxygen to burn at a particular point in time.

So, a flammable mixture on the other hand is the reactant mixture which can burn without additional oxidizer or fuel; that means, it has adequate amount of fuel and oxidizer already in the mixture itself. So, if I isolate a system, I do not feed anything to this; oxidizer or fuel.

Under that condition, it has sufficient amount of fuel and oxidizer to burn. So, what is the lean limit? That is lean value of Φ which is less than 1 or rich value of Φ which is more than 1 which will accomplish ignition. Do you understand?

So, for example, if this is say 0.6 for some particular fuel air mixture. This may be 2.1 something like that. So, only under this condition it will burn, if Φ is reduced less than Φ_{lean} or Φ is increased more than Φ_{rich}, the ignition will not take place or we cannot have flame propagated propagating through such a mixture. So, these are called limits, flammability limits.

The equivalence ratio on the lean side and equivalence ratio on the rich side, they are called limits or boundaries of the flammable mixture. Now, a reactant mixture based upon the type of fuel obviously and oxidizer; you can have pure oxygen or air or something; so, different type of oxidizer will have different flammability limits. That means, they are flammable only in certain proportions and under certain conditions of temperature and pressure.

So, when you increase its temperature, this limit will widen. Unburned gas temperature say I say my temperature is 298 K, reactant temperature; so, reactant temperature is 298 K, then I have a particular value for Φ_{lean} and Φ_{rich}.

When I increase, say this is not my temperature, now I increase this to say 350 K, then this will widen. I can burn it in a slightly leaner and slightly richer conditions also. So, based upon this temperature, pressure and the fuel type; instead of methane, if I add hydrogen, then it will be wide limits, it will be presenting to us.

So, based on the reactant mixture I say. The flammability limits are determined based upon the type of fuel, type of oxidizer; then, the temperature and pressure, that we have to understand. The heat released during the combustion will also vary. Obviously because if you have a lean to rich and rich to again further rich etcetera, you will have the heat release which is going to be changing that is the obviously known to us.

Now, how will you determine these limits of flammability? That will be determined using standard test procedures, there are lot of standards. Normally, what they do is they take a vertical pipe say normally 2 inch in diameter or say 50 mm, 50 mm in diameter. So, I will write diameter here, 50 mm diameter and have the spark.

So, they can give spark here; this is spark and this is filled up with reactants; so, filled up with the reactants. So, this will be very long, say maybe 2 meters something like that; obviously, we have to provide length to this and the reactant mixture is supplied here.

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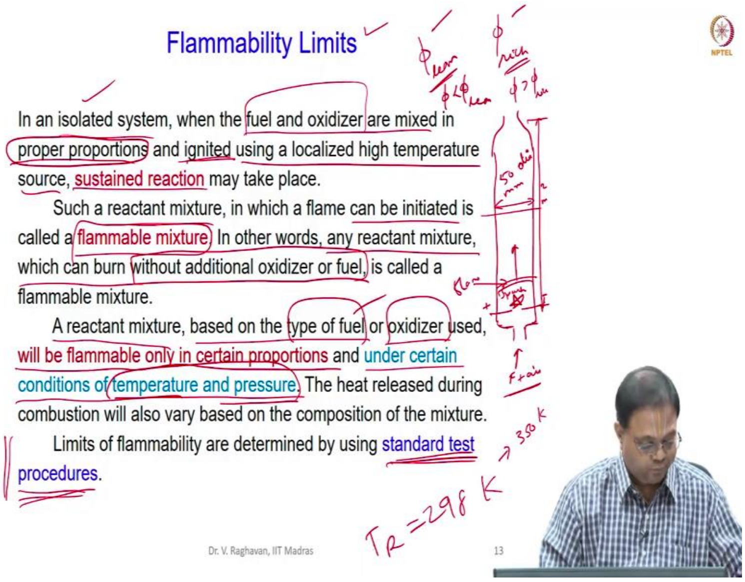

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So, I say fuel plus air is supplied here, you can have any reactant. Please understand that fuel plus oxygen also you can supply; any reactant at any temperature, you can make and supply this and once this is filled up, then give a spark here and see whether a flame is formed. So, once you give a spark, a flame forms.

So, this is the flame and it propagates through the mixture. So, this test procedure basically calls for the flame to propagate at least half of the distance, half of the height. So, once it is ignited at the bottom, it should proceed to half of the height of the column. Once it proceeds like that, then the mixture is said to be flammable.

So, the standard test procedures calls for a vertical tube say 50 mm in diameter which is filled up with reactant at a particular condition, any Φ value or T_u value, pressure etcetera. Then it is ignited from the bottom and flame has to form and propagate; the flame forms, but only propagates to a few millimeters and extinguishes.

That is not the case. At least the flame should propagate till half of the height of this tube. So, some procedures are there, once this test is passed, then that mixture, you can say may be 0.6 is now passed. So, that is within the flammability limit.

Now, if we take equivalence ratio of 0.3 and do this, the flame may not be initiated at all. So, 0.35 may ignite; 0.3 may not ignite. So, the 0.35 is called the lower flammability limit or equivalence ratio corresponding to the lower flammability limit. Similarly, when we make the mixture richer and richer, at an equivalence ratio of say 2.5, it may not ignite after that. So, 2.45 may ignite; 2.5 may not ignite. So, the upper flammability limit is set as $\Phi = 2.5$. So, this is the way you determine the flammability limits.

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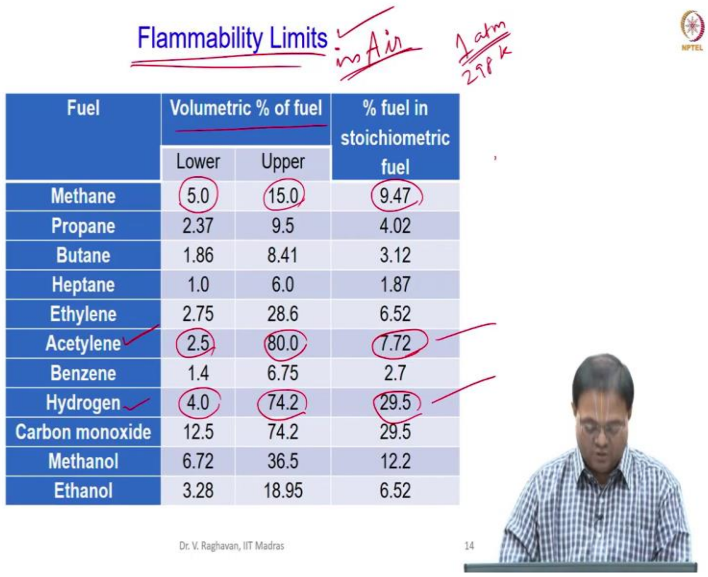

Flammability Limits in Air

1 atm
298 K

Fuel	Volumetric % of fuel		% fuel in stoichiometric fuel
	Lower	Upper	
Methane	5.0	15.0	9.47
Propane	2.37	9.5	4.02
Butane	1.86	8.41	3.12
Heptane	1.0	6.0	1.87
Ethylene	2.75	28.6	6.52
Acetylene	2.5	80.0	7.72
Benzene	1.4	6.75	2.7
Hydrogen	4.0	74.2	29.5
Carbon monoxide	12.5	74.2	29.5
Methanol	6.72	36.5	12.2
Ethanol	3.28	18.95	6.52

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And this is the table of flammability limits of several fuels, important fuels are given here and please understand that here we have not presented it as a function of Φ; but I have given volumetric percentage of fuel, when I have a fuel air mixture and this is for the air, flammability limits in air. If it is in oxygen, it will be different. So, this is in air and one more thing is this is conducted at one atmospheric pressure and 298 K, that is the initial condition of the reactants.

Now, what is the flammability limit? For methane, when I say 5% and 15%; that means, methane will burn when 5% of methane by volume is present in the reactant mixture. If it is 4.5%, it will not burn; it will not ignite. And the upper side, so now, starting from 5%, you make 6%, 7%, 8% increase the fuel content rich 15%, it may ignite, add more say 0.5% percent more, 15.5% of methane, it will not burn.

So, the lower flammability limit 5% corresponds to the volumetric percentage of fuel; that means, in the mixture 5% by volume is occupied by the fuel that will burn. Similarly, in the mixture if 15% is occupied by the fuel, that will burn. Stoichiometric value is 9.47% that is also given here to understand, where the stoichiometry lies.

So, if for the methane-air mixture to be stoichiometric, 9.47% of methane should be present in the mixture, that is stoichiometric mixture. So, decrease that. So, lean level, it may go to 5%; rich level, it will go to 15%. So, that is the this. So, for several fuels, I have listed here. But some important thing we can note, for example, Acetylene. 2.5% of acetylene by volume in the mixture will burn, it will ignite.

Similarly, 80% of acetylene will also ignite. So, this is very wide flammability limits. So, you have a very rich fuel-air mixture that is 80% of this mixture volumetrically is acetylene, it will burn. Similarly, 2.5%, only very low amount of acetylene, it will ignite, such a wide range of flammability limits are very dangerous. Similar thing is exhibited by the hydrogen also; 4% to 74.2% that is another important fuel.

But others are not so bad, you can see they are not in a narrow range of flammability limits; but for this acetylene, you can see this stoichiometry is only 7.72%, but you can see the rich; it goes to very rich values and burns. Similarly, here 30%, around 30%, 29.5% is the stoichiometric volume percent of fuel in the mixture of hydrogen and air. But you can see the wide flammability limits are exposed here. These are all very active.

This means that storage of these fuels acetylene and hydrogen etcetera are not easy. Because you know any small leak of air or small leak of fuel to the atmosphere can cause a problem. A small leak of air, so that say 20% of the volume is now air, then the acetylene will become a flammable mixture now.

Similarly, when some small amount of acetylene leaks through this area, then you can see 2.5% of this volume is acetylene. Then, we are going to be unsafe, that is what this indicates. So, this is very important to understand the flammability limits and manage of a storage accordingly. So, this is very important characteristics. Flammability limits is another important characteristic of the premixed mixture.

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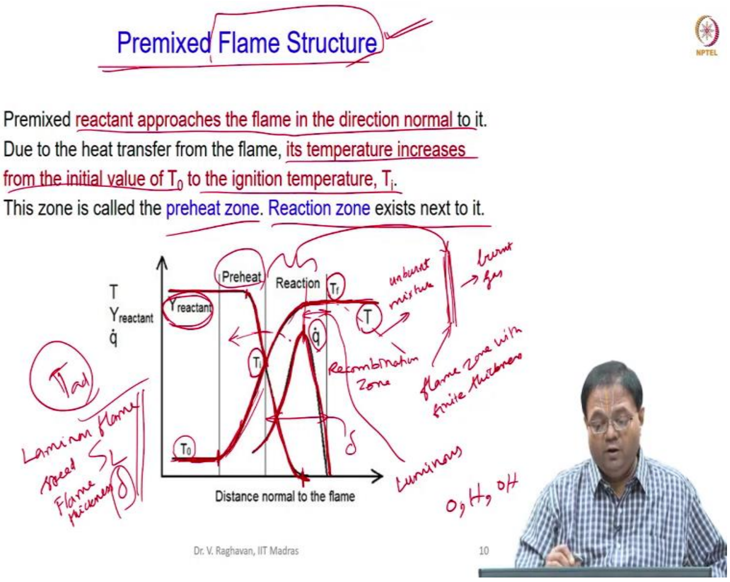

Premixed Flame Structure

Premixed reactant approaches the flame in the direction normal to it. Due to the heat transfer from the flame, its temperature increases from the initial value of T_0 to the ignition temperature, T_i. This zone is called the preheat zone. Reaction zone exists next to it.

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Now, we are interested in finding two things; the structure basically, also we are interested mainly to find this S_L value, associated with this is the thickness of the reaction zone which is called δ; so, del. So, laminar flame speed and flame thickness and T_{ad}; T_{ad} is thermodynamically you can find this. So, this is not a problem. Then the structure, basically we are interested in the structure. So, these are the important things.

Measuring of S_L is possible. This is actually based upon the equipment etcetera; we have some range; but measuring the flame thickness is not so easy. But anyway, optically we can try to do that or you can also measure the temperature across this and try to arrive at this. In the profile if you know, based upon the profile, we can get approximate thickness of the flame, gradients etcetera and so on.

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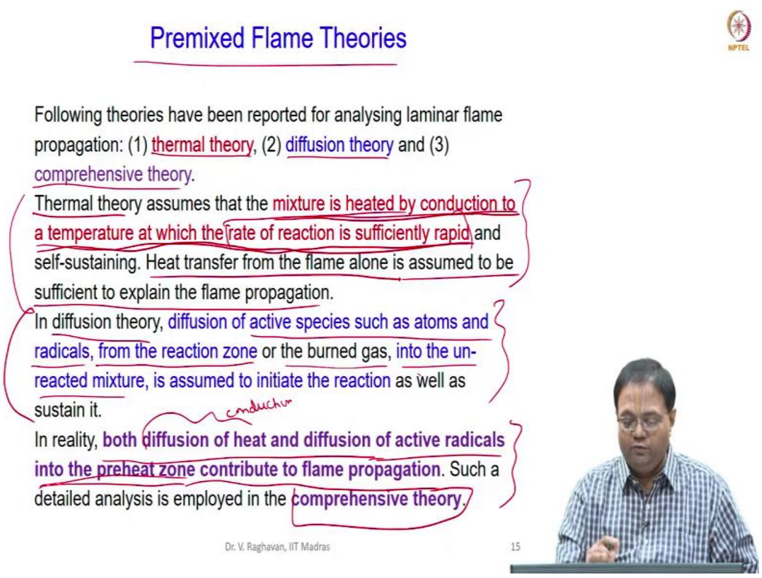

Premixed Flame Theories

Following theories have been reported for analysing laminar flame propagation: (1) thermal theory, (2) diffusion theory and (3) comprehensive theory.

Thermal theory assumes that the mixture is heated by conduction to a temperature at which the rate of reaction is sufficiently rapid and self-sustaining. Heat transfer from the flame alone is assumed to be sufficient to explain the flame propagation.

In diffusion theory, diffusion of active species such as atoms and radicals, from the reaction zone or the burned gas, into the un-reacted mixture, is assumed to initiate the reaction as well as sustain it.

In reality, both diffusion of heat and diffusion of active radicals into the preheat zone contribute to flame propagation. Such a detailed analysis is employed in the comprehensive theory.

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Now, theoretically can we do this? That is the next attempt, what we are going to make. Here, we will see some premixed flame theories. There are three types of theories which have been reported by the researchers. First one is called thermal theory, second one is called diffusion theory and third one is the comprehensive theory.

So, thermal theory; what it does is it assumes that the mixture is heated by conduction to a temperature at which rate of reaction is sufficiently rapid. So, we have already seen in the preheat zone as the unreacted mixture comes in, reactant mixture comes in, at a particular point due to the heat transfer from the reaction zone, the temperature of the mixture increases and reaches a particular value called ignition temperature.

So, that is what is told here. When the mixture is heated by conduction to a temperature at which the rate of reaction is sufficiently rapid. When the temperature of the reactant reaches the value of T ignition then the reaction rate become sufficiently higher, because you know that the reaction rate is exponentially dependent on temperature.

So, as the temperature slightly increases at a particular value, you will see a sharp increase in the reaction rate. So, what is that temperature? That temperature is nothing but the ignition temperature. So, in the preheat zone, the temperature increases to that value and where the reaction rates are sufficiently large, that is the starting point of the reaction zone.

Now, in the thermal theory, the heat transfer from the flame alone is assumed to be the important aspect and that is enough, they say that is enough for explaining the flame propagation that is it. So, they do not need to consider the radical, we have already seen that some radicals are also transferred from the reaction zone to the preheat zone and they cause the initiation step, chain initiation step etcetera.

But thermal theory says that we need not assume those things, we will just say by measuring the temperature. We can see and tell what is happening about the flame propagation.

Exactly opposite to this is the diffusion theory, in which it says that the active species such as atoms and radicals, H, OH, CO etcetera which are transported from the reaction zone or the burned gases into the unburned zone or the premixed zone, that is the main cause. Without radicals, the initiation step cannot be formed.

Once the initiation steps are formed and complete like at the start of the reaction zone, then only reaction can proceed, within the small thickness, it may complete. So, that is the concept here. It is called diffusion theory, but in practice we need both; so, both diffusion of heat and diffusion of active radicals.

So, diffusion of heat, when I say its conduction and diffusion of active radicals into the preheat zone. Preheat zone which is just before the reaction zone contribute to the flame propagation. So, this is called comprehensive theory.

But it is easily said when you go for this, we have to numerically solve the problem; we cannot theoretically solve the problem, that is what the problem is. So, here also it is not easy to solve the problem theoretically. So, the thermal theory this is actually going to be very useful for us to understand certain things.

So, basically the factors which are going to affect the S_L value and the δ value etcetera, that can clearly come out of thermal theory itself. So, that is what we are going to see now.

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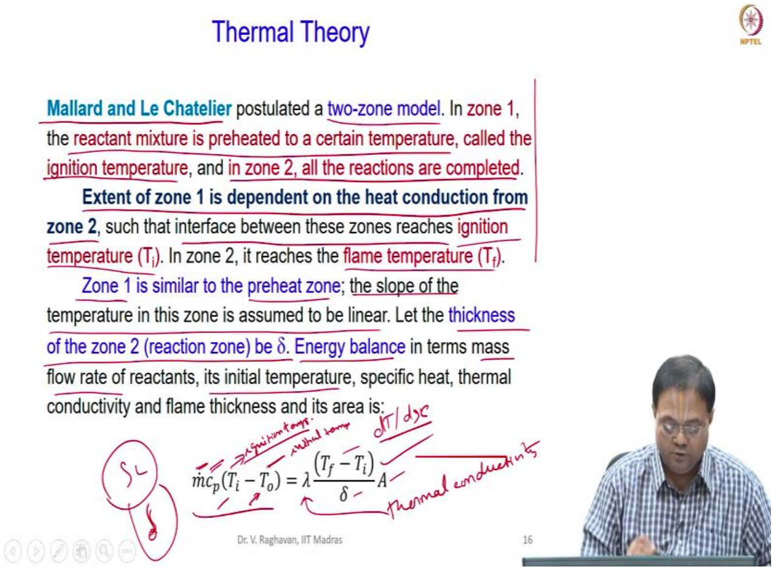

Thermal Theory

Mallard and Le Chatelier postulated a two-zone model. In zone 1, the reactant mixture is preheated to a certain temperature, called the ignition temperature, and in zone 2, all the reactions are completed.

Extent of zone 1 is dependent on the heat conduction from zone 2, such that interface between these zones reaches ignition temperature (T_i). In zone 2, it reaches the flame temperature (T_f).

Zone 1 is similar to the preheat zone; the slope of the temperature in this zone is assumed to be linear. Let the thickness of the zone 2 (reaction zone) be δ. Energy balance in terms mass flow rate of reactants, its initial temperature, specific heat, thermal conductivity and flame thickness and its area is:

$$\dot{m}c_p(T_i - T_o) = \lambda \frac{(T_f - T_i)}{\delta} A$$

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Now, thermal theory basically several people have done it. Initially done by Mallard and Le Chatelier; same concept. They have said there are two zones in this, two-zone model. The zone 1, where the reactant mixture is preheated to a certain temperature, that temperature is called ignition temperature that is also formed by them. So, that is the zone 1 which we called preheat zone, the same thing they are called in zone 1.

The next is the reaction zone, where all the reactions are completed, that is called zone 2, what we call reaction zone it is zone 2. Now, similarly the extent of zone 1 is dependent on the heat conduction from the zone 2, where the temperature starts to rise, that is the point where the start of zone 1 or the preheat zone prevails. Such that the interface between these zones reaches the ignition temperatures; these two zones that is the end of the preheat zone, start of the reaction zone or end of zone 1, start of zone 2 should be at ignition temperature T_i. Heat release occurs at the reaction zone so that the flame temperature reaches; the temperature reaches the value of flame temperature T_f in the reaction zone. So, already we have discussed this.

So, same thing was assumed in the long before; flame thing same concept was given. So, once we know this, we can very easily find the transport of the fuel and the rate at which it is transported etcetera we can find the propagation velocity and so on. So, how we are going to do this? Some assumptions have to be made, let us make it. Because any theoretical calculations, we need to make simplifying assumptions.

So, because the problem what we have in the hand is non-linear, we have to make some simplifying or non-complicated assumptions, so that we get some theoretical solution, which at least indicate to us the factors which are going to affect the values of S_L and δ. So, as I told you zone 1 is similar to the preheat zone.

But, if you go back and see this temperature profile, you can see this is the non-linear profile here. Non-linear, a slight nonlinearity is there in the profile. But what they have assumed here? In the theory, what they have assumed is the temperature, slope of temperature in this zone is linear; the nonlinearity is not there, only its linear.

So, that is the assumption made, that is fine; it is almost linear. Now, again the thickness of the zone 2 reaction zone is δ. So, that is what we are interested to find also. So, that is there. So, now let us apply the energy balance. How will you do it?

Energy balance in terms of mass flow rate of the reactants $\dot{m}$, then the specific heat of the reactants and the initial temperature that is T_0, T_i is the ignition temperature and this is the initial temperature. So, initial temperature of the reactants is T_0; initial and the ignition temperature which is going to be attained at the end of the preheat zone, that is ignition temperature T_i.

So, the heat required for the incoming reactants which has the mass flow rate of $\dot{m}$ and specific heat of c_p to rise its temperature from the initial temperature of T_0 to T_i that is the heat which is transported from the reaction zone or the zone 2 to zone 1. How it is transported? By conduction; that is thermal conductivity λ, then reaction zone thickness δ, this is dT/dx, temperature gradient and area.

So, that the heat conducted from the reaction zone to the preheat zone is used to heat the reactant which is flowing in at the rate of $\dot{m}$, which is having a specific heat of c_p and its temperatures rises from T_0 initial temperature to the ignition temperature T_i. So, this is the simple heat balance which we have written and please understand that this dT/dx is approximated as T_f - T_i in the reaction zone divided by δ, which is reaction zone thickness.

Since, the thickness is very small, this is valid basically. So, this is one of the important assumptions made. So, you write this equation. So, how will you incorporate other things and find the value of S_L that is what is important now. S_L and we have to find the value of δ. These are two values which are going to determine.

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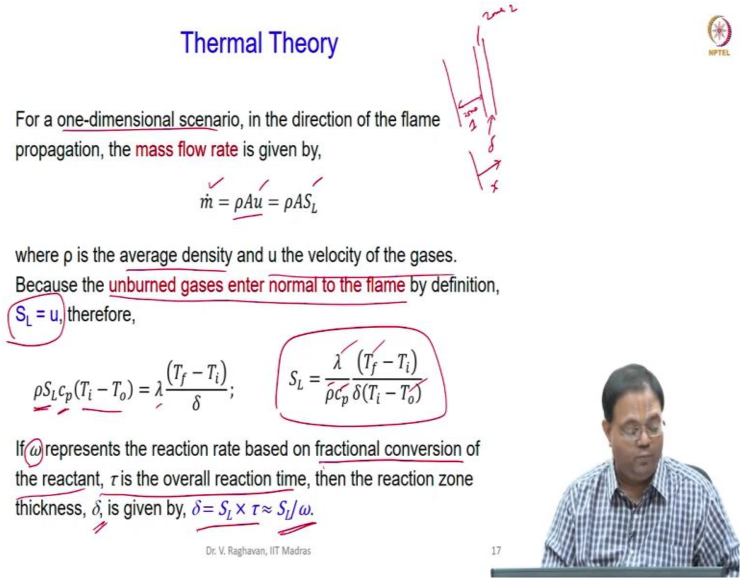

Thermal Theory

For a one-dimensional scenario, in the direction of the flame propagation, the mass flow rate is given by,

$$\dot{m} = \rho A u = \rho A S_L$$

where ρ is the average density and u the velocity of the gases. Because the unburned gases enter normal to the flame by definition, $S_L = u$, therefore,

$$\rho S_L c_p (T_i - T_o) = \lambda \frac{(T_f - T_i)}{\delta}; \qquad \boxed{S_L = \frac{\lambda}{\rho c_p} \frac{(T_f - T_i)}{\delta (T_i - T_o)}}$$

If ω represents the reaction rate based on fractional conversion of the reactant, τ is the overall reaction time, then the reaction zone thickness, δ, is given by, $\delta = S_L \times \tau \approx S_L / \omega$.

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So, now, so one-dimensional scenario; that means, there is a flame zone and we have a preheat zone. So, this is δ and this is the zone 1 thickness, zone 1 and this is the reaction zone, zone 2 and one-dimension. So, you are interested in see starting from here.

So, this is x direction; so, one-dimensional scenario. The direction of flame propagation; so, we can say the flame propagates in the negative x direction or flame is stationary and reactants are fed in the positive x direction or flame propagates through the unburned gases and so on.

So, the mass flow rate of the reactant is ρAu. Here, u is the unburnt gas speed. So, ×Au or we can say $\rho A S_L$ because if the flame is stationery the reactants are going to be fed to the flame at the velocity of small u. If the flame moves through that reactant mixture, it will propagate at a velocity of S_L. So that means, S_L should be equal to u, in one-dimensional scenario.

So, ρ is the average density. Please understand average density, why we are saying because there is unburned and burnt temperature or there is a temperature gradient basically. Due to which the density will vary. So, we can take average; so, $(T_0 + T_i)/2$ or

$(T_i + T_f)/2$. So, some average temperature, we can take and evaluate the density, u is the velocity of the gases. So, that will be determined by the flow rate of the reactants.

So, unburned gases enter normal to the flame, you can say $u = S_L$ or $S_L = u$. So, substitute these things here $\rho S_L A$, A is there; it will cancel eventually here. Here also there is A; right hand side also there is A, so that cancels. So, c_p, then $T_i – T_0 = \lambda(T_f - T_i)/\delta$. So, that is the flux here. So, A cancels basically.

So, from this S_L can be determined by this equation. But please understand that this equation has two unknowns; S_L as well as δ; δ is also not known to us. Even very importantly T_i also is not known to us. See adiabatic flame temperature, we can somehow calculate using some thermodynamic principles. You know T_0; λ, ρ, c_p, there are some way to calculate that for the mixture. So, T_i, we do not know much, we do not know what is the value of T_i.

So, either we have to make some assumption here or there is no other way to calculate, we have to make an assumption here. Similarly, apart from that we have two more unknowns that is S_L which is going to be calculated over δ. So, somehow, we have to eliminate this. So, how to do this? First, we try to eliminate δ; but let us say ω is the reaction rate.

So, fractional conversion; say for example, if 1 kilomole fuel is present, fractionally when it converts say, α moles are is consumed. So, fractional conversion, we know some kmol/m^{3}s that is called fractional conversion. If we know, we can also write it in kg/m^{3}s, that if we know, then S_L.

So, the reaction time is τ, then the flame has a thickness of δ that is defined as S_L, the flame propagation time is τ; that means, if the reaction is going to occur within a time τ, the flame has to propagate a distance of its thickness δ within that time. So, we can say $\delta = S_L \times \tau$, but τ is $1/\omega$. So, S_L/ω that is the δ.

So, now I have eliminated δ, I am going to put S_L for that; S_L/ω for that. So, now please understand here, if ω represents the reaction rate based on fractional conversion of the reactant, basically assuming one unimolar reaction. So, reactants giving product something like that, then τ is the overall reaction time, then the δ can be found by multiplying S_L and τ or S_L/ω because $\tau = 1/\omega$.

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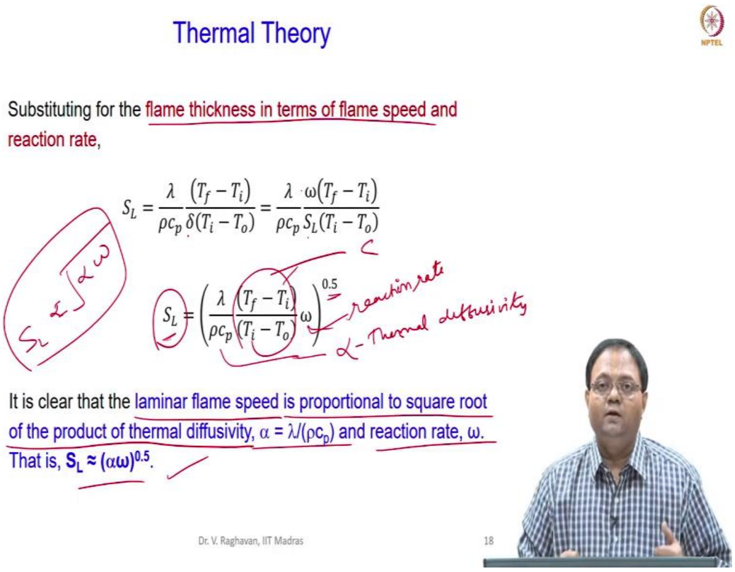

Thermal Theory

Substituting for the flame thickness in terms of flame speed and reaction rate,

$$S_L = \frac{\lambda}{\rho c_p}\frac{(T_f - T_i)}{\delta(T_i - T_o)} = \frac{\lambda}{\rho c_p}\frac{\omega(T_f - T_i)}{S_L(T_i - T_o)}$$

$$\boxed{S_L \propto \sqrt{\alpha\omega}}$$

$$S_L = \left(\frac{\lambda}{\rho c_p}\frac{(T_f - T_i)}{(T_i - T_o)}\omega\right)^{0.5}$$

C

reaction rate

α - Thermal diffusivity

It is clear that the laminar flame speed is proportional to square root of the product of thermal diffusivity, $\alpha = \lambda/(\rho c_p)$ and reaction rate, ω. That is, $\mathbf{S_L \approx (\alpha\omega)^{0.5}}$.

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Now, substituting the flame thickness in terms of flame speed; we got this. δ is substituted by S_L/ω that is all. So, now you get this. Please understand that this is not so accurate, again please understand that there is some assumption which we are going to make with respect to T_i and omega we know. But, we can say that this T_f - T_i and $T_i – T_0$ are of the same order; so that means, that this will become a constant now for us.

So, we can say $S_L = (\lambda/\rho c_p)\omega$ into some constant which is very close to unity, let us say. So, that power 0.5. So, laminar flame dependence is got. $S_L \approx (\alpha\omega)^{0.5}$. So, this is what is this $\lambda/\rho c_p$, thermal conductivity divided by density into specific heat this is nothing but the α, thermal diffusivity and this is the reaction rate.

So, now S_L is proportional and I can say S_L α $\sqrt{\alpha\omega}$, ω is the reaction rate. So, these are the factors which influence this, that is what the thermal theory gives. The factors which are going to influence this laminar flame propagation.

So, it is clear that the laminar flame speed is proportional to the square root of the product of thermal diffusivity α, $\lambda/\rho c_p$ and the reaction rate ω. So, that is very important. So, this is the thermal theory and it may not give us absolute value.

So, now please understand that by empirical correlations, we can fit this may be taken as a constant and these properties can be evaluated at some average temperatures and similarly, the reaction rate also can be evaluated at the average temperatures, then we can get a correlation, empirical based correlation for S_L. Now, knowing the dependency of S_L; so now, we can confidently say that S_L will be dependent on under root alpha into omega; that is what the thermal theory provides us.