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

# Lecture - 36 Laminar Diffusion Flames - Part 4 Estimation of laminar flame speed

(Refer Slide Time: 00:14)

Factors Affecting SL	NPTEL
$S_L \approx (\alpha \omega)^{0.5}$ .	
Since $\omega$ is exponentially dependent on temperature, S <sub>L</sub> has similar	
dependence: $\left[ \left( E_{a} \right) \right]^{1/2} \gamma_{b} \qquad \qquad$	
$S_L \approx \left[ exp\left( -\frac{R_u T}{R_u T} \right) \right]$	
For an <u>n<sup>th</sup> order reaction</u> , the reaction rate depends on pressure, p,	
as $(p^{n-1})$ Therefore, dependence on S <sub>L</sub> on p is expressed as,	
$(S_L) \approx \left(\frac{1}{b}p^{n-1}\right)^{1/2} \approx (p^{n-2})^{1/2} \qquad \qquad$	
S <sub>1</sub> is independent of p for n = 2. Experiments show that S <sub>1</sub> presents	
a decreasing trend with increasing pressure up to 10 atm.	and the second
Dc.V., Raghavan, IIT Madras. 19	

Now, let us see in detail. So, this when I say  $\alpha$  and  $\omega$ , we all are normally interested in finding the temperature, pressure dependence and maybe  $\Phi$  dependence which we have already seen. So,  $\omega$  reaction rate is exponentially dependent on the temperature. So, S<sub>L</sub> will have the similar dependence.

So, you know  $\omega$  is written as A×exp(-E<sub>a</sub>/R<sub>u</sub>T) into concentration of reactants power some order. Say, order n. So, now this exponential dependency of  $\omega$  will also say this, this power half, so exponential dependency is this term basically, this is temperature term; we also can have a term called T<sup>m</sup> here.

Now, if that is present, we can also add  $T^{n/2}$  here because  $S_L \alpha (\omega)^{0.5}$ . So, the exp(- $E_a/R_uT$ )<sup>0.5</sup> $T^{m/2}$ , but this term is not going to affect the  $S_L$  so much as this exponential term.

So,  $S_L$  has an exponential dependency on temperature since  $\omega$  has that. Then, let us consider n<sup>th</sup> order reaction. Most of the reactions are second order reactions, but let us

first consider here general  $n^{th}$  order reaction. So, the reaction rate of  $n^{th}$  order reaction depends upon pressure as  $p^{n-1}$ .

So, as the pressure varies, the reaction rate will vary to as  $p^{n-1}$ . So that means, where  $\omega$  is affected by p.  $\omega$  is the function of p comma T,  $\omega(p, T)$ ; we have seen the T dependence here, pressure dependence here. Now, similarly  $\alpha$  will be  $\lambda/\rho c_p$ .

So, all other variables,  $\lambda$ ,  $c_p$  etcetera will not vary much with these pressures; but  $\rho$  will vary. So,  $\rho = p/RT$ . So,  $\rho$  will vary with pressure. So, that term is here. So, this is p. So,  $S_L$  varies as  $(1/p) \times p^{(n-1)0.5}$  which is nothing but  $(p^{n-2})^{1/2}$ . So,  $S_L$  varies with pressure as for the n<sup>th</sup> order reaction. Please understand, for n<sup>th</sup> order reaction, it varies as  $(p^{n-2})^{1/2}$ . But many reactions are second order in nature; that means n equal to 2. So, if you put 2 here p power 0; that means,  $S_L$  may not depend much on pressure. However, some small dependency is shown by the experiments which show that  $S_L$  presents a decreasing trend with increasing pressure up to 10 atmospheres, where the experiments are conducted. So, this you have to remember. So, temperature is the one which is going to mostly affect the  $S_L$  value and pressure slightly affects it.

(Refer Slide Time: 03:42)



Now, the thermal theory gave us; see here the from thermal theory, we got these points, for example this.

### **Thermal Theory**



۲

Important conclusion from thermal theory is  $S_L \approx \sqrt{\alpha \omega}$ , is proportional to under root  $\alpha$  which is thermal diffusivity and  $\omega$ , product of  $\alpha \omega$ . And based upon that, the other factors temperature pressure etcetera which influence, we have already seen how the temperature is going to be affect. See since the strong dependence on  $S_L$  and temperature is present here, so  $S_L$  follows the temperature which is also seen already.

As you can see that the adiabatic flame temperature variation which was shown here in this slide, which presented a variation with equivalence ratio producing a maximum value at a slightly richer condition for methane air flames.

(Refer Slide Time: 04:29)



(Refer Slide Time: 04:41)

#### Laminar Flame Speed Variation



(\*)

Similarly, its laminar flames also poses the typical variation producing a maximum at the slightly richer point. So, temperature dependence of  $S_L$  is clearly illustrated and equivalence ratio that affects the temperature, it affects the  $S_L$  also in the similar manner. (Refer Slide Time: 05:02)

Laminar Flame Speed Variation	NPTEL
For $CH_4$ and $C_3H_8$ , the equivalence ratio at which $S_1$ becomes a maximum is around $1.09$ and for $C_2H_2$ , it is around $1.2$ . For $H_2$ , it around $1.8$ and for CO, it is around $2$ , implying that a richer mixture is required for attaining the maximum flame speed for these fuels. One important point to note here is that the occurrence of the	
maximum adiabatic flame temperature for hydrogen-air mixture	
same as that of methane. However, the maximum flame speed occurs around an equivalence ratio of (1.8.)	
This is due to the variation of thermal and mass diffusivities, or	
their ratio called Lewis number, Le, with the composition of the	ale.
reactant mixture.	
Dr. V. Raghavan, IIT Madras 9	

But if you take hydrogen type of fuel, there are some discrepancies which we have noted here due to the highly non unity Lewis number and temperature dependent property values. Now, we are going to go for what is called simplified analysis in which what we are trying to do is we will assume several things try to pose equations; but anyway, use the energy equation to find some quantitative equation or expression for  $S_L$  and  $\delta$ , that is laminar flame speed and the flame thickness.

So, here also we are assuming one-dimensional flame propagation, that is a simplified approach has been given by or reported by Professor Spalding. Lot of assumptions have

to be done for any simplified analysis, where we are not going to use say numerical approach, only theoretical approach is used, then simplified assumptions have to be made.

So, one-dimensional constant area duct in which the flame is propagating, then constant pressure, the pressure variations are not much. Steady propagation which is almost true, steadily the flame propagates. Then, what we are not going to see is take into account thermal radiation; radiation heat transfer is not taken into account.

Then, the thermal diffusion which is called Soret effect, it is not going to be taken into account. The secondary effect, second order effect which is due to Soret effect the mass diffusion takes place; thermal gradient drives the mass. Similarly, due to the mass transport or concentration gradients, energy flux will be transported that is Dufour effect. Then, viscous dissipation etcetera which are work done due to high speed flows, which is not take into account. Obviously, it is not significant at all. So, these are negligible. Again, which is not true always. Lewis number is 1, but we are assuming that.

Similarly, another assumption is specific heats of all the species are the same, that is  $c_{p,i}$  is constant; i can be any 1 to N. There is no variation in the  $c_{pi}$ 's and they are constant values. So, they will not vary with temperature also;  $c_{pi}$  equal to constant means at a given temperature  $c_p$  of CO<sub>2</sub> may be equal to  $c_p$  of N<sub>2</sub> or  $c_p$  of CH<sub>4</sub>.

So, that assumption is made because of little difference at a given temperature. But with temperature, the variation is not taken into account because we are going to take some average temperature and calculate these values. So,  $c_p$  values are constant. The mixture  $c_p$  also is a constant because there is mixture  $c_p$ ;  $c_p$  is a single variable here that is also held as constant.

Then, single step reaction is assumed here. Please understand that premixed flames are kinetically controlled. So, in a simplified assumption, we cannot invoke all the equation, chemical reactions and elementary reactions. So, we assume a single sub reaction here. But understand that in a kinetically controlled process, we cannot assume the reaction to be single step to get accurate results.

But in a simplified analysis, to get some order of values, magnitude values, we can invoke the single step reaction; but we cannot eliminate a chemical reaction at all. So, please understand at least a finite rate reaction is necessary. So, we cannot assume that the reaction rate is infinitely fast, that cannot be assumed, that is the finite rate which is imposed to the chemical reaction. It may not be a very detailed mechanism, but at least it should take into account some finite rate at which the reaction takes place. That means, if we assume the infinitely fast reaction, then the flame thickness will approach 0 value.

So, in order to avoid that, in order to impart some finite thickness for the flame, the reaction rate also is assumed to be at a finite rate, which is due to a single step reaction. So, now governing equations; mass conservation d/dx; x is the direction of the propagation,  $d(\rho u/dx) = 0$ .

So, mass is conserved.  $\rho u = \rho_u S_L$ . Please understand,  $\rho u$  is the product of density and velocity at any point which is should be equal to the velocity at which the unburnt reaction mixture approaches the flame in the normal direction. So,  $S_L$  is velocity there or the speed.

(Refer Slide Time: 10:08)



Now, for the reaction 1 kg of fuel + s kg of oxidizer  $\rightarrow$  (1 + s) kg of products PR. The conservation equations are written in the one-dimension without the unsteady term.

$$\rho u \frac{dY_F}{dx} = \frac{d}{dx} \left( \rho D \frac{dY_F}{dx} \right) + \dot{\omega}_F'''$$
$$\rho u \frac{dY_{Ox}}{dx} = \frac{d}{dx} \left( \rho D \frac{dY_{Ox}}{dx} \right) + \dot{\omega}_{Ox}'''$$
$$\rho u \frac{dY_{PR}}{dx} = \frac{d}{dx} \left( \rho D \frac{dY_{PR}}{dx} \right) + \dot{\omega}_{PR}'''$$

So, this is the diffusion term; convective term, diffusion term and the source term. So, please understand one more thing, this D is also taken as constant here and same for all the variables. So, that assumption is also made. So,  $\rho D$  is constant.

So, you can write this equation. But please understand this, these equations are still nonlinear, we can see the we cannot eliminate the reaction rates; the reaction rate is important for this particular thing. But by using these three equations, we can simplify the energy equation. So, simplified energy equation is given here. This is simplified. So, we have already seen how to simplify energy equation in the previous chapter governing equations for the reacting flow.

$$\rho u c_p \frac{dT}{dx} = \frac{d}{dx} \left( \lambda \frac{dT}{dx} \right) - \dot{\omega}_F^{\prime\prime\prime} \Delta \mathbf{h}_c$$

So, we have taken a single like one-dimensional equation energy equation and applied the conservation equations to find this equation. So, this we have derived actually in the previous chapter. Please understand the species equations are not going to be used in this; but the species equations are used to get this value. So, this energy equation which is simplified. We have enough equation to solve the problem.

So, here what we are trying to say is convection of the thermal energy  $\rho$ u that is the mass flux in to c<sub>p</sub>dT/dx that is the enthalpy will be equal to the conduction of heat and the heat which is released due to the combustion that is  $-\dot{\omega}_F''$ , it is a negative quality because consumption of fuel. So, negative and negative is positive.

So, this becomes a source term for us multiplied by  $\Delta h_c$ .  $\Delta h_c$  is the heat of combustion which is positive. So, these equations are used to derivate the simplified energy conservation equation. Now, we are going to solve the energy equation in the zone. (Refer Slide Time: 12:50)



Now, what is the zone we are assuming? The zone where this is the x direction, here this is the x direction; at x = 0 and this is  $x = \delta$  and this is  $x \rightarrow -\infty$  and  $x \rightarrow +\infty$  on either side.

Now, as the reactant approach at this point, at x = 0, its temperature starts to increase and at the end of this reaction zone,  $x = \delta$ , its temperature reaches the flame temperature.

So, single zone we are assuming; reaction zone with the thickness of  $\delta$  is taken and single zone is assumed, where the unburnt reactants with the temperature of  $T_u$  approaches from  $-\infty$ , at this point, it is at  $x = -\infty$  to x = 0, it approaches.

Then at that point of x = 0, it simply just starts to increase and finally reaches the flame temperature  $T_f$  at the end of the reaction zone given by  $x = \delta$ . So, the boundary conditions for this is as  $x \rightarrow -\infty$ ,  $T = T_u$  and dT/dx = 0, because its flat. As  $x \rightarrow +\infty$ ,  $T = T_f$  and dT/dx = 0. So, these are the boundary condition; second order equation.

This is a second order equation. Due to this conduction term, the second order equation we get. To solve this, we need boundary conditions in surrounding  $-\infty$  to  $+\infty$ . Again, you can split into several zones and do this, we will see that. Now, the mass flux  $\rho u$  which is arising due to the mass conservation and this thickness of the reaction zone, this  $\rho u = \rho S_L$ . So, that  $S_L$  itself is a unknown quantity.

Similarly, this thickness is unknown quantity, they are eigenvalues. Other problem; so, this problem. We are stating this as an eigenvalue, we are going to solve this. Please understand as I already told that species conservation equations are not used here, they were actually used to simplify the energy equation and write this in this form. Energy equation is written in this form due to by the help of these equations. We have already seen that.

(Refer Slide Time: 15:29)



Now, integrate the energy equation. So, just integrate each term and in the limit, we have to put. For example, in the limit of  $-\infty$ , T will have a value of T<sub>u</sub> and  $+\infty$ , it will have a

value of  $T_f$ . So, the first term, the convective term is integrated  $\rho uc_p = \text{constant}$ ;  $\rho u$  is constant as a result of mass conservation and we have assumed  $c_p$  is a constant.

So, based upon that  $T_u$  we have to do integration in the limits. Similarly, the diffusion term, the conduction term will be written like  $\lambda dT/dx$ ; dT/dx = 0 at  $-\infty$  and  $+\infty$ , both. So,

we have to apply this. And source term, which is this,  $\Delta x$  (which is constant)  $\times \int_{-\infty}^{+\infty} \dot{\omega}_F''$ .

Now, evaluating the integrals first, first term here in the left hand side  $\rho uc_p(T_f - T_u)$  and this term becomes 0, the first term in the right hand side becomes 0 and this term is retained here. So,  $-\Delta h_c \int_{-\infty}^{+\infty} \dot{\omega}_F''' dx$ . So, please understand that in this analysis, we are not

eliminating the source term, that is the reaction rate term is very important.

So, we have to implement a finite rate of reaction so that we get this value of  $\delta$  evaluated properly. So, the limits of the integral right hand side can be changed from x to T because know we do not know see, we know that the reaction rate, the rate of conservation of fuel etcetera strongly depends on temperature. So, we can calculate the temperature the limits which are in the x now can be changed to T and dx can be changed to dT.

(Refer Slide Time: 17:28)

(\*) Integration of Energy Equation The reaction rate is valid only between  $T_u$  and  $T_{f}$ . If  $dT/dx = (T_f - T_u)/\delta$ , then  $dx = [\delta/(T_f - T_u)]dT$ . Therefore,  $\rho u c_p (T_f - T_u) = -\Delta h_c \frac{\delta}{(T_f - T_u)} \int_{\sigma} \phi_F^{\prime\prime\prime} dT$ The integral in the right hand side is the average reaction rate:  $\frac{1}{(T_f - T_u)} \int_{\tau}^{T_f} \dot{\omega}_F^{\prime\prime\prime} dT = \left( \overline{\omega}_F^{\prime\prime\prime} \right) \xrightarrow{\Lambda} \mathcal{N}^{\prime\prime}$ Dr. V. Raghavan, IIT Madras

So, for that the reaction rate is valid. So, we can see that only in the zone between x = 0 and  $x = \delta$ , where T is in between T<sub>u</sub> and T<sub>f</sub>, the reaction rate has some meaning. So, in this zone, we can write dT/dx as  $\Delta$ T, that is T<sub>f</sub> - T<sub>u</sub>/ $\delta$ .

So, when you write this, then we can write dx as  $\delta/(T_f - T_u)dT$ . So, substitute that, you get this. Left hand side remains the same;  $\rho uc_p(T_f - T_u) = -\Delta h_c \times \delta/(T_f - T_u) \int_{T_u}^{T_f} \dot{\omega}_F''' dT$ .

Now, you can note that this 1/ (T<sub>f</sub> - T<sub>u</sub>)  $\int_{T_u}^{T_f} \dot{\omega}_F'''$  dT is a average reaction rate. The reaction

rate is very low at  $T_u$ ; its very high at  $T_f$ ; within this range. It is some average value. If you integrate the reaction rate which is lower at  $T_u$  and very high at  $T_f$ , you get an average reaction rate which is defined as  $\overline{\omega}_F^m$ , that is the average reaction rate.

So, that we can substitute now. Average reaction rate, we can calculate using an average temperature. Obviously,  $(T_f + T_u)/2$ , we can use to calculate  $\omega_F$ . So, you know expression for  $\omega_F$ . So, that is Aexp(-E<sub>a</sub>/R<sub>u</sub>T), you have to put this into concentration of fuel or reactant power n. So, this is the reaction rate. Now, you have to put the T here, you have to put  $T_{average}$  here to get this value.

(Refer Slide Time: 19:34)



MPTEL

Incorporating the average reaction rate, the equation is written as,

$$\rho u c_p (T_f - T_u) = -\Delta h_c \delta \overline{\omega}_F^{\prime\prime\prime}$$
 (A)

To handle two eigen values, the energy equation is again integrated in the limits of  $x \rightarrow -\infty$  and  $x = \delta/2$ . In this regime, the reaction rate is assumed to be zero. T at  $\delta/2 = T_a = (T_f + T_u)/2$  and  $dT/dx = (T_f - T_u)/\delta$ .



So, once you get this value, you can substitute this, the right hand side can be simplified and I now write the right hand side,  $\rho uc_p(T_f - T_u) = -\Delta h_c \delta \overline{\omega}_F'''$ .

This equation, the  $\delta$  comes there. So, this remains. So, S<sub>L</sub> is unknown,  $\delta$  is unknown. So, two eigenvalues are still there in this equation.

So, what we do is we have to integrate this equation one more time, but now with the different limits. When you see this, initially what we integrated? When we integrated the

energy equation, we considered limits as minus infinity to plus infinity. Now, we once again integrate to get 2 eigenvalues.

So, one more eigenvalue I have to get. So, I integrate this equation energy equation, now with the limit which is from minus infinity to  $\delta/2$ . So, half of the reaction zone. So, this is  $\delta/2$ . So,  $-\infty$  to  $\delta/2$ , let us try to integrate now. So, that is what I am going to do now.

So, to handle two eigenvalues, the energy equation is again integrated within the limits of extending to  $-\infty$  to half of the reaction zone and generate. So, eliminate one variable. For that, I am trying to do this. So, in this regime, why I am choosing this regime because I am assuming that, in this regime no reaction will take place.

So, it is a one-zone model. But I know that some pre-heat should have happened. So, now, what I am assuming that in this zone  $-\infty$  to x equal to half of this reaction zone thickness, I assume that the reaction rate may not be so high because of the low temperatures prevailing because exponentially the reaction rate increases with temperature increase.

So, when the temperature is between  $T_u$  to the middle portion of the reaction zone, there is not much increase in the temperature; even though, it is linearly varying. So, in this regime, the reaction rate is assumed to be negligible or 0. So, now what is the temperature value?

T, we know at  $-\infty$ , T = T<sub>u</sub> and dT/dx = 0, these two boundary conditions I know. But what are the boundary conditions at  $\delta/2$ ? T at  $\delta/2$  is average temperature because linear profile, here linear profile.

So, in this point temperature will be average of these two;  $T_f$  and  $T_u$ . So, I say that as T average,  $T_a = (T_f + T_u)/2$ . So, temperature at  $\delta/2$ , the second boundary is this. Similarly, dT/dx can be assumed to be  $(T_f - T_u)/\delta$ . So, that is the temperature gradient slope; slope is constant know. So, that is the slope which we have in this.

So, that dT/dx at that point  $\delta/2$  is the slope of the entire curve which is  $T_f$  and  $T_u$  by  $\delta$ . So, if we use this, now we integrate the equation; the source term disappears because in this range of regime  $-\infty$  to  $\delta/2$ , it is easy to approximate the reaction rate to be 0 because temperatures are low enough, exponentially temperature increases.

So, at low temperature, the reaction rates are low; temperature increases to a higher value, exponentially the reaction rate increases. So, keeping in mind, the source term is absent. Now, you can see the limits of the left hand side will be  $T_u$  to  $T_{average}$ .

Similarly, dT/dx = 0 to  $dT/dx = (T_f - T_u)/\delta$ . So, now, when you do this, you get the equation which connects  $\rho_u$  and  $\delta$ .  $\rho u \delta/2 = \lambda/cp$ , so that is what we get here.

#### Solution



So, that you can use here this and if we connect A and B, we will get the solution. So, now, you know  $\rho_u S_L$  and  $\alpha$  is  $\lambda/\rho c_p$  and now, the heat of combustion is nothing but the mass flow rate of the heat.

So, 1 kg of fuel + s kg of oxidizer  $\rightarrow$  1 + s kg of product. So, 1 + s kg of products into its c<sub>p</sub> into temperature difference T<sub>f</sub> - T<sub>u</sub> that will be the heat flow due to the flow of the products. So,  $\Delta h_c$  is nothing but that. So, if you substitute, you get the expression for S<sub>L</sub> which is this.

So, here the negative is because of this  $\dot{\omega}_{F}^{"'}$  is negative. So, this is a positive quantity. So, again, the same thing we are getting that is  $(\omega \alpha)^{0.5}$ , but other terms are there which we can evaluate now. We know the fuel, I know what is s value, what is  $\rho_{u}$  value etcetera and I can find the  $\alpha$  and  $\dot{\omega}_{F}^{"'}$  at average temperature.

So, some value of  $S_L$  can be determined based upon the reaction rates and these quantities. So,  $\delta$  can be written in terms of  $\alpha$  and  $S_L$  like  $2\alpha/S_L$ . So, these are the two quantitative expressions which we have got from the simplified analysis. Still, you please understand that this is not so accurate, but it will give some quantitative results.

In the previous thermal theory that  $T_i$  was used, so in the two-zone model, the ignition temperature cannot be like eliminated. So, for that some assumptions have to be made. Here, the zones are combined and actually what we are trying to do here is we are saying that the  $T_i$  approaches  $T_f$ , that is what we are trying to do here and try to get the values. So, here the dependency of  $S_L$  on  $\sqrt{\alpha \omega}$  (average reaction rate) is clearly present.