Lecture – 54
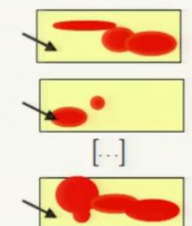**Turbulence-Chemistry Interaction (contd…)**

Okay, welcome back. And let us continue the discussion on the mixture fraction kind of model. So, we have looked at the Burke Schumann kind of flame and what happens when we have single step reversible and irreversible chemistry and whether we have an infinitely fast chemistry or finite rate of it. We have seen how it changes and we establish and simple equation for mixture, mass fraction, and species mass fraction and the temperature as a function of z.

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And then finally we got the relationship between the enthalpy and mixture fraction. Now look at the mixture fraction in turbulent flame. Let say we start with an RANS kind of framework. So, we have mixture fraction or other this is our instantaneous which is sort of affected due to the turbulence and then you divide that into 2 components. One is the mean and one is the fluctuation.

So, this is mean + fluctuation. And the mean value, one can find out it could be ensemble average. This is a Reynolds average for number of sample and Z_n, this we have repeatedly discussed again and again that how we can obtain the mean values and all these things. So, now, when you talk about the reacting system, one of the important aspect is that we have to consider the density weighted mean.

And the density weighted mean for mixture fraction and would look like $\langle \rho Z \rangle / \langle \rho \rangle$ and then the fluctuation in density weighted average would be $Z - \bar{Z}$. So, this is what we will be using for density weighted system.

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Now, once we use this density weighted average in RANS framework, our mixture fraction equation will look like that we have convection term, ancillary term, convection term and diffusion term. And as we have already seen mixture fraction equation is free from any chemical source term, but due to these emerging we come across a term which is the scalar flux term and that remains unclosed.

So, this term is sort of unclosed and this is one of the term what requires to be closed and using ready and diffusion assumption. The simplest way one can close is that it is a:

$$-\bar{\rho} D_t \frac{\partial}{\partial x} \tilde{Z}$$

So, this is one of the best ways and as long as there is no counter diffusion present, this works for large number of flows. So there is no issue associated with that kind of situation. Now then when you use this, the closure approximation in this particular equation, this will come down to this equation under RANS framework, uncertain term, and convection term. This is the total diffusivity. So this $D + D_t$ is effectively the effective diffusivity. So, these molecular and D_t is the turbulent diffusivity which is closed from using the eddy viscosity and the turbulent Schmidt number.

So, then this equations in RANS framework looks completely close, and we can now solve this transport equation, and then find out the evolution of z which in turn allowed to calculate the species and temperature profile inside the domain.

Now, how do you obtain this mean property? So that is an important question, because we have transformed our system from the local space to mixture fraction space. So, these for example, this is our flame front. Let us say this is our flame front and this is flame normal analysis. So, our transport equation is in physical space, this is z equation, but our and is free from source term and we are not solving mass fraction and all these things.

So those equations, the equation for the mass fractions and temperature they are solved in this normal space, which is essentially the mixture fraction space. That means they are taken as a function of z and they are solved there were individual mass transfer equation and that variance and in one dimensional front is calculated. And it is done at the pre-processing stage or pre-computed and store those information in a form of table.

Now, while we are solving in the physical space this evolution of the mixture fraction using that information we can use that table to find out a particular species and temperature. This is similar to the approach that we have discussed for premixed flame like and progress variable kind of approach and what it allows that you require some probability density function, which is again and shape of the distribution would be assumed which is called presumed, which we have seen in the BML model another model presumed PDF. So, one can now look at that the

probability density function approach also has 2 different categories. One is the presume shape PDF and which is also applied in both laminar premixed flame and non-premixed flame. And that is another one is the transported PDF approach. Transported PDF is also theoretically applicable to both the regime, but it is more reliable or it requires tuning for each of this regime to use properly.

But dimensional wise transported PDF expenses are quite expensive. It is a heavy dimensional and that is why you solve in a hybrid approach where you solve mean profile in the Eulerian framework. And the transport equations of the problem density function is solved in the Lagrangian framework. Compared to that when you look at this presumed PDF, it is much simpler, much easy to implement and it is quite faster.

Now, what happens? So, our mean species mass fraction will be integrated over equilibrium mass fraction, which is a function of z as I explained here, and that probability distribution function or density function fz dz. And favre averages mass fraction would be equilibrium mass fraction, which is a function of z and favre average density function. So, the favre average distribution function would be $\frac{\rho(z)}{\bar{\rho}} f_z(z)$.

Now, if you look at this z, which comes in this is your oxidizer z_0, this is fuel z_1 they come in. So at this particular location, if you look at the probability distribution function. At this location, this will look like this because this is more close to the oxidizer side. You can see some distribution of z. Here you can see some distribution this is a Caussian distribution.

So, there are different probability distribution function in the field using these distribution function and the information of mass fraction which is a function of z one can find out the favre average mean mixture fraction.

So, if you go to the equilibrium flamelet model under turbulent condition, what one has to do at any location x, you can find out the mean values and then you can find out the mixture fraction or the using the information of the mixture fraction, you can find out the mass fraction or the favre average mass fraction using the equilibrium information of z and the probability distribution function.

So, this is what you get as a final result in the turbulent flame. And similarly, favre average temperature which will be the temperature is a function of z so, it includes the effect of turbulent movements of flame position but not finite rate kinetics because our equilibrium information is like this our oxidizer comes to at z stoichiometric. This is fuel, this is oxidizer and our temperature can go like this. So, this is our temperature.

Otherwise stoichiometric so, these are all Y_{fuel}, $Y_{oxidizer}$ and T. There function of z only and z solved using that and probability density function we get this. And $\rho_1/\bar{\rho}$ can be equated 0 to 1, 1 by which is also a function of these which will be the connection between.

Now, this is called the assumed shape PDF method or presumed shape PDF method. So, in turbulent flow that z the mixture fraction which is in the physical space that is fluctuating under the effect of eddies. Now the probability density function of Z(x) has to be found. Now, once we assumed that PDF, the shape of the PDF is assumed but mean and variance have to be calculated. So, this is one important thing.

So, the equation along with your mean mixture fraction, one has to look at the variance. It is a similar approach in a way one can think or correlate with the z equation or level set approach that we discussed in the frame of premixed flame. When you want to bring in this effect of turbulence and the interaction with the small scale structure and the large scale structure or different regime, you have to solve the variance of the G equation.

Similarly, here we have to also solve the variance of the mixture fraction. So, you have 2 system, one is the mean mixture fraction and the variance which is written as g. So, these are the 2 transport equation that we get, one for the mean mixture fraction, which is free from against source term and the D effective is $D + D_t$ and for the variance equation, we get the similar up to this ancillary term, convection term and diffusion term but then we get an production of z variance and that dissipation.

So, these are the 2 term which we come across when you derive the mixture fraction variance. And this guy is dependent on the mean mixture fraction and because this is a gradient of mean mixture fraction and that is square and the dissipation term depends on some timescale ratio

C_φ and the turbulent isolation that allow some sort of a ratio between these 2 that. So, that is what one can get.

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Now, it comes to the point how you define your PDF function or probability density function, which is in presumed shape. So, the one which is quite popular in literature, the definition is in gamma function. So, the $f_z(z)$ is defined as:

$$\tilde{f}_z(z) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} z^{a-1}(1-z)^{b-1}$$

Now here we use the value of mean mixture fraction and the variance b is defined by $\left(\frac{a}{\tilde{Z}} - a\right)$ and a is:

$$a = \tilde{Z}\left[\frac{\tilde{Z}(1-\tilde{Z})}{g} - 1\right]$$

So, we need information of both Z and Z variance, which we get from the transport equation or other in the physical plane physical space solution of transport equation.

Turbulent Non-Premixed combustion

Assumed shape PDF method / Presumed shape

In turbulent flow Z(x) is fluctuating.
The probability density function (PDF) of Z(x) has to be found.
Assumed PDF method:
  the shape of the PDF is assumed but
  mean and variance have to be calculated.
Mean mixture fraction $\tilde{Z}$ and variance $\widetilde{Z''^2} \equiv g$ of mixture fraction
are obtained from modeled transport equations

$$\frac{\partial \tilde{Z}}{\partial t} + \frac{\partial}{\partial x_i}\left(\overline{\rho}\tilde{u}_i\tilde{Z}\right) = \frac{\partial}{\partial x_i}\left(\overline{\rho}D_{eff}\frac{\partial \tilde{Z}}{\partial x_i}\right) \qquad D_{eff} = D + D_t$$

$$\frac{\partial g}{\partial t} + \frac{\partial}{\partial x_i}\left(\overline{\rho}\tilde{u}_i g\right) = \frac{\partial}{\partial x_i}\left(\overline{\rho}D_{eff}\frac{\partial g}{\partial x_i}\right) + 2\overline{\rho}D_{eff}\frac{\partial \tilde{Z}}{\partial x_i}\frac{\partial \tilde{Z}}{\partial x_i} - C_\phi \overline{\rho}\frac{\varepsilon}{k}g$$

                                                production   dissipation

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And now you can see in the physical space as these guys are evolving, because they have answered the effect they have convection. They have diffusion and G also has some source term. So, their evolution is not going to be very unique, they would be quite scattered there would be effect of turbulence and once you find or get that evolution pattern using that you can find out this b at every location in the flow field.

Turbulent Non-Premixed combustion

Example shapes of the β-function

$$\gamma = \frac{a}{\bar{Z}} = \frac{\tilde{Z}(1-\tilde{Z})}{g} - 1$$

Different shapes of the mixture fraction PDF
found in different regions of the flame

Dirk et al.

CH4

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And then you can estimate that probability density function for that value of Z and Z variance and then using that you can find out the mean things. So, this is one of the example which has been taken from a delta burner where it is a laboratory scale natural gas burner. This is where CH$_4$ is burning and you can see these and beta function and the gamma (γ) is:

$$\gamma = \frac{a}{\tilde{Z}} = \frac{\tilde{Z}(1-\tilde{Z})}{g} - 1$$

And it is a different shapes of the mixture fraction PDF found in different region of the flame. So, you have this region and other region and you can see the difference shape. So, that means this distribution function since this is a strictly a function of Z variance and $\tilde{Z}$ they are evolution will dictate how this object is going to look like.

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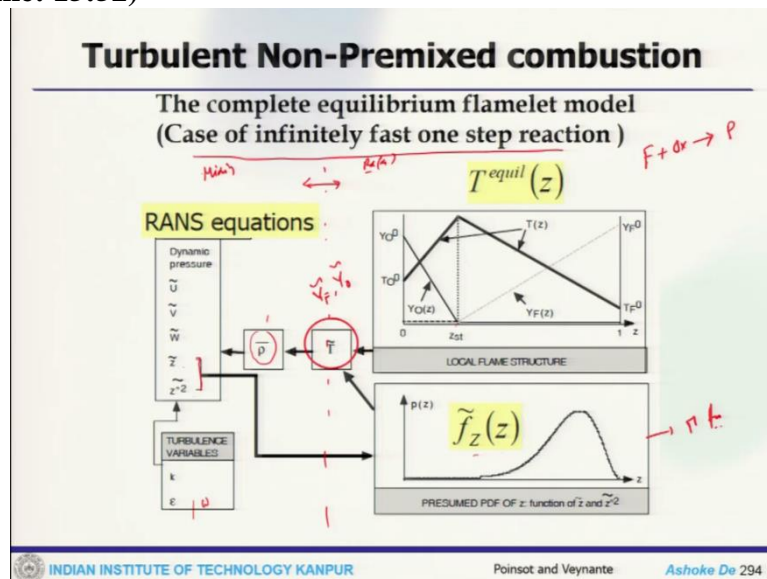
So, this is an important information one can have now, to complete this part of the discussion on the equilibrium flamelet model. So, what you can see this is a case for infinitely fast one step reaction that means, Fuel + oxidizer to get product. This is infinitely fast reaction. So, this whole thing will give you a complete idea about how the whole things are handled in RANS framework.

So, in Eulerian phase or framework you saw pressure, velocity component, mixture fraction and variance, and which also in connection with turbulence variables with the k, epsilon and omega. So, all these mean proves you solve in the Eulerian field. Now, using this information of Z and Z variance, you can find out the probability density function which will look something like that, which is essentially a gamma function.

So, that gamma function you can estimate and you get in for a particular location, particular instant of the time and this would look like this. Now, from our equilibrium calculations, we have a local flame structure, where oxidizer becomes 0 at Z stoichiometric, fuel will become

0, because this will vary from 1 to 0 oxidizer rule. Well, so, this is a profile of oxidizer. This is a profile of fuel and this is a profile of temperature which is strict function of Z.

Now, we use this information of local flame structure and probability density function we get the mixture temperature. Also we can find out Y_F and Y_u. Using this, we estimate the mean density. Now, these mean density has an impact or effect of the temperature due to reacting system and that is fed to the Eulerian framework. Now again the Eulerian system is solved and next instant of time depending on these values we do the same thing. So, these goes in a loop. So, that means that coupling between these so you can think about there are 2 stages of the whole business or 2 system this split into 2 parts. One is this mixing part and this is the reaction or equilibrium kinetic part and they are connected between these to the mean density. Because mean density is the term which actually connects these Eulerian mean profit calculations because that has all these density and other side is the local flame structure.

So, that is fairly give you an idea how your equilibrium assumption or equilibrium flamelet model works and that is simple enough to be implemented.

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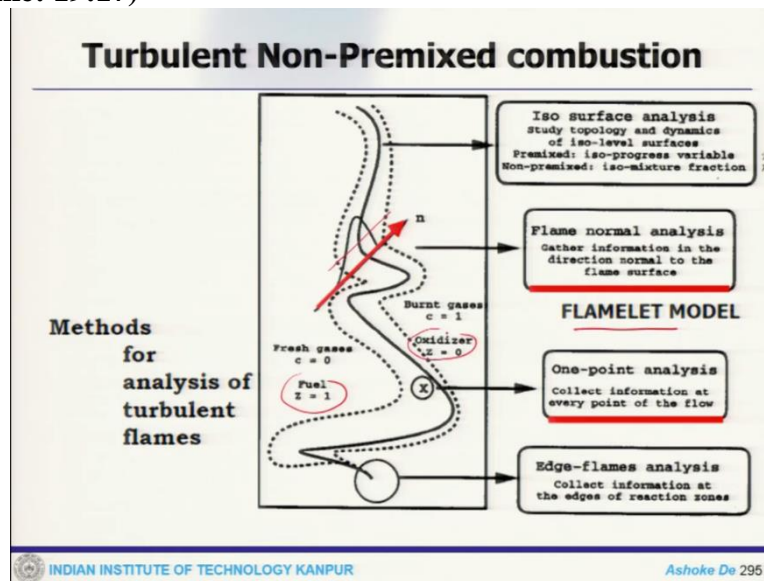
Now, coming back to this picture, this is what our flamelet model where it belongs, it is a flame normal analysis that means you actually convert these things along these normal space. Now, we are discussing about system of non-premixed flame.

So, that is what one can use. Now, something more about this mixture fraction this we have already that fraction of the mass present locally. And this is how the equation looks and fuel inlet of the air and fuel. Now, the question here is that can it be expressed in terms of measurable quantities?

That is what is quiet important that how do you estimate these things in terms of some quantities which are miserable. Now, we use the definition of the Lewis number. So, the Lewis number for individual species would be:

$$Le_i = \frac{D_h}{D_{im}}$$

This D_{im} is mixture thermal diffusivity, species diffusivity with respect to mixture. Now, it is:

$$D_{im} = \frac{1}{Le_i} \frac{\lambda}{\rho C_P}$$

Now, this will be the species mass fraction equation on steady term, convection diffusion source term. Now convert that thing and use the information of the Lewis number we get this. So, it is basically these particular term is kind of replace to it this.

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Now, once we do that, what happens? So it taken situation again that single step kinetics with irreversible reaction, fuel, oxidizer and product. Now we find out the scalar without the source term. So that means, Z_{un} which is defined as:

$$Z_{un} = v_O W_O Y_F - v_F W_F Y_O$$

This is how it is defined. What we can see now.

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We multiplied this particular equation this is what we got using the Lewis number you multiplied with first $v_O W_O$ and this is the fuel mass fraction or mass transfer equation and the

second one which is the oxidizer mass transfer equation. So, we multiply this one with the fuel $v_F W_F$ this is $v_O W_O$ from this one to this one if we subtract. So, you get:

$$\frac{\partial \rho Z_{un}}{\partial t} + \overline{\nabla}.(\rho \overline{v} Z_{un}) = \overline{\nabla}.\left(\frac{1}{Le}\frac{\lambda}{C_P}\overline{\nabla}.Z_{un}\right)$$

So, that the diffusivity of the fuel and oxidizer are equal stoichiometric values are. So, this case, we are assuming that D_F and D_O are same.

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Now we construct the mixture fraction. So, this is a normalization to ensure the boundary condition now, this is the oxidizer side, this is the fuel side up to stream and this would be:

$$Z = \frac{Z_{un} - Z_{un,2}}{Z_{un,1} - Z_{un,2}}$$

Z_{un} is:

$$Z_{un} = v_O W_O Y_F - v_F W_F Y_O$$

So which you can write:

$$Z_{un} = v_F W_F (s Y_F - Y_O)$$

$Z_{un,1}$ is:

$$Z_{un,1} = v_F W_F (s Y_{F,1} - Y_{0,1})$$

And,

$$Z_{un,2} = v_F W_F (s Y_{F,2} - Y_{0,2})$$

So what we get:

$$Z = \frac{s Y_F - Y_O + Y_{0,2}}{s Y_{F,1} + Y_{0,2}}$$

When inlet is 1 is fixed to fuel inlet that is other one side is oxidiser inlet. So get an expression for Z which uses the mass stoichiometric ratio, which is:

$$s = \frac{\nu_O W_O}{\nu_F W_F}$$

Now, if you have detailed chemistry, then how do actually construct this mixture fraction. So, this is a very known formula or it was derived by professor Bilger. This is a scalar without source term, but the species molecules which are component or has elements of atoms C, O, H and N. Let μ_{kj} denotes the number of atoms of element k in molecule of species j. So, we go by the element mass fraction definition which is for a element k of a mixture of species is given by:

$$Z_{e,k} = \sum_{j-1}^{n_i} \mu_{kj} \frac{W_{e,k}}{W_j} Y_j$$

Now, the whole idea is that elements are not destroyed by chemical reactions. Therefore, the element mass fractions are scalar quantities without chemical source term. Now in the diffusion species is described by the diffusion coefficients relative to the mixture and the diffusivity of all contributing species are equal, the element mass fraction also has the same Lewis number. So this is an important observation. In general case of non-equality Lewis number of the element mass fraction has more complex diffusion properties dependent on species gradients. So, that is what it has.

Now, we can have a stream. Stream 1 and stream 2, and we can normalize that thing. So, Z_k is an elemental k – at second stream the elemental k by the first stream to the second stream, now in the diffusivity of all species same. So, the mixture fraction based on different elements are also become identical. So, that is another thing that would happen.

Now, thing is that how do we extract the mixture faction from the experimental data set. So, there are Raman - Rayleigh measurements which provide the simultaneous data on major species, but that is not sufficient for a good approximation of the element mass fraction. So, what happens that, one linear combustion of element mass fraction can be used like that unnormalized mixture fraction:

$$Z_{un} = \gamma_C Z_{e,C} + \gamma_H Z_{e,H} + \gamma_O Z_{e,O} + \gamma_N Z_{e,N}$$

And then we can normalize this Z unnormalized at second stream to unnormalized at the first stream to second stream. So this is at the stream 1 and stream 2. So, this should be $Z_{un,1}$, this is $Z_{un,2}$. So one can define the stoichiometric conditions for hydrocarbon combustion and inlet nitrogen. So it would be:

$$\frac{Z_{e,O}}{W_{e,O}} = 2\frac{Z_{e,C}}{W_{e,C}} + \frac{1}{2}\frac{Z_{e,H}}{W_{e,H}}$$

And the proposition the Bilger proposed these different things. So, γ_C is $\frac{2}{W_{e,C}}$, γ_H is this is as per Bilgers definition. There is a nice article on this how you can find out this mixture fraction or elemental mixture fraction like this. γ_O would be $\frac{-1}{W_{e,C}}$, γ_N is 0.

Now, once you use these information here, you finally get unnormalized stoichiometric Z is 0 even in the presence of differential diffusion. So, you can see not necessarily you have to actually assume that equal diffusivity even for non equal diffusivity, you get these things to be 0. So, we will stop the discussion here today and continue these mixture fraction based things in details in the next lecture.