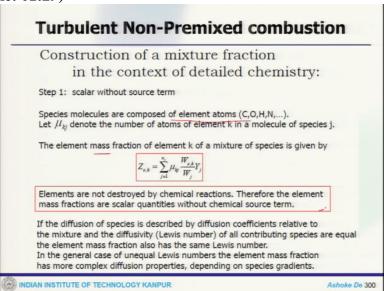
## Turbulent Combustion: Theory and Modelling Prof. Ashoke De Department of Aerospace Engineering Indian Institute of Technology, Kanpur

## Lecture - 55 Turbulence-Chemistry Interaction (Contd...)

Welcome back. So, let us continue the discussion on the non-premixed combustion, where we are during the discussion of the mixture fraction based basically the concept scalar kind of approach and what we have looked at it, when we have an equilibrium assumption and then we solved the main flow field and through there, we assume the PDFs are the probability density function and at the different location in the domain you have a different probability and then from that using the local flame structure.

Where we assume the equilibrium assumption that means, fuel, oxidizer and temperature all these would be Stickle function of the mixture fraction and also we have looked at that example from a perspective of a single chemistry and then, using that local flame structure along with the PDF we get the mean profiles like for temperature, species mass fraction, like fuel and oxidizer. And then the connection between the Eulerian frames are the main flow field is done through the density and that is where we stopped.

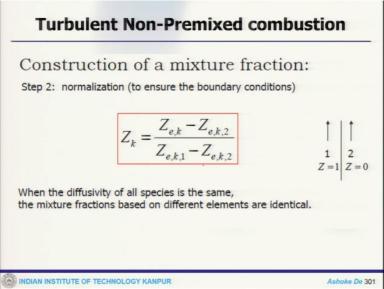
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And now will quickly go through the elemental mixture fraction, which is for a detailed chemistry and then from the elementary mixture fraction. So, that is what we have already looked at it, you have each species composed of some elements C, O, H, N, then at the element

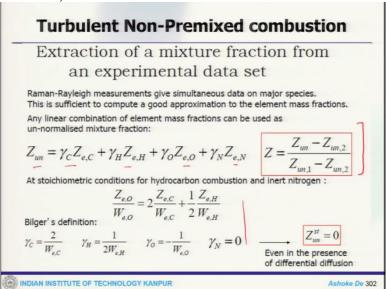
level. You can define the elemental mass fraction like this, and the elements are not destroyed by chemical reaction. The mass fractions also can be obtained, now, then for this, we can normalize it actually for these both the terms, we can normalize the mass fractions using that.





And then finally, what do you get the un-normalized mixture fraction, which is written in terms of carbon atom, hydrogen atom, oxygen atom, nitrogen atom and this is how you get the mixture fraction using those un-normalized mixture fraction and then you use this Bilger's information to get these things.

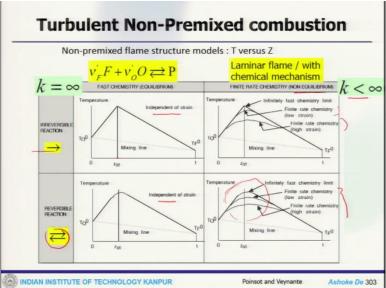
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So, this is how you can using the elemental concept also you can find out these things. Now, moving ahead. We already have looked at this where you have a single step chemistry it could

be reversible or non-reversible and then if we just consider the reversible case, you have 2 limits, and one is the first chemistry live in where it will immediately become equilibrium.

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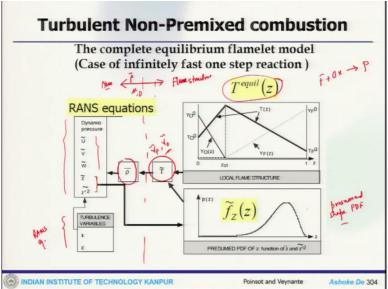
That means, what will happen at the stoichiometric all the fuel will get consumed and oxygen also get consumed and you will get the maximum temperature which is becoming independent of strength. And this is strictly for irreversible reaction with the fast chemistry limit that means, if I look at my fuel, from there, the fuel will become zero here, oxygen will become zero here and the temperature will go up. At the same time, if you have a finite rate chemistry limit which is a non-equilibrium situation and k is less than infinity.

The temperature, this is the peak which you get from the infinitely fast chemistry assumption. And these are the situations where you get the finite chemistry for low strain and finite chemistry. And you can see the temperature profile goes smooth and having, I am showing some sort of a current this is a representative flow can be obtained for a particular fuel using a particular standard one can get this information.

That is not quite difficult to obtain, one can write a small few lines, MATLAB code and even get that thing. Now, when you use the reversible situation, you can see when the equilibrium limit where the fast chemistry assumption is there, the temperature does not go peak, it takes a smoother profile. This is still independent of strain. And then when you take the finite rate effect for different strain condition, you see the profile variation.

And one important thing to be noted here is that the infinitely fast chemistry limit which is an equilibrium limit always produces the maximum temperature and when you have actually strain effect that means the realistic flame they do expose to the strain effect and the temperature comes down. Now, if this is in a situation where you are fuel + oxidizer to product this is infinitely fast one step reaction.

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So, If we complete the equilibrium flamelet model, this is what we solve the main flow field and along with the turbulence information, so, this could be RANS equation. For the turbulence model, it could be k omega, k realizable, k upsilon, it could be anything not necessarily it has to be k upsilon and then using this information, the mixture fractional variance, we can estimate the probability density function. So, this is in presumed shape PDF.

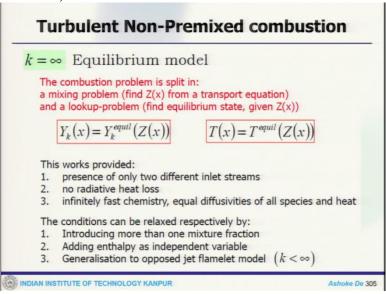
So, this you obtained and from the equilibrium limit, you have all this information like oxygen, fuel and temperature. They are strictly function of Z these two you combine get them in mean profile also you can get mean profile for fuel and oxidizer and also you obtain the density. This is an important term because this is actually the density if you look at it this side. So that is the density is the term which actually and also if you have a temperature dependent viscosity and diffusivity, they made the handshaking between these mean field equation to the flame structure or local flame structure.

So, what you can see that means is sort of splitted in 2 different segment one you said okay, it is only mixing control and you solve for all these and then using the local information of the

flame structure with the presumed shaped PDF, we close the terms and the mean profiles, density and the transport property, which will again go back and be used in this mean for profile equations.

We close the terms and the mean profiles, density, viscosity and all these are used. That is how they are a back and forth information are in text place and the whole calculation progresses. Now, our equilibrium model, which is an situation where you have  $k = \infty$ , that means it is where fuel gets burnt, the oxygen gets to also burnt there would be temperature peak.





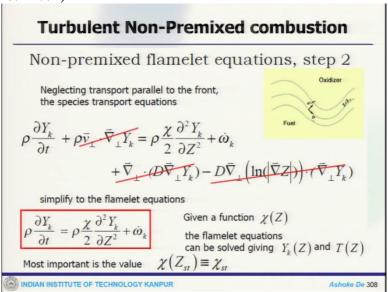
So that is everything sort of and this is our JDST this is fuel, this is Ox and this is temperature. So they get actually burnt, and you can see these things this is now the whole thing it is splitted into 2 problem, first one is the mixing problem of Z(x), where Z(x) and variants the transport equation is solved. And second is the lookup problem from equilibrium state given is that means this local flame calculation, one is the mean field calculation and is the local flame structure calculation.

So, when in the local flame structure, you have this information where your temperature would be the function of Z(x) and your mixture fraction is also going to be the function of Z(x). So, this again was provided. If it is only two stream problem, this works very nicely. There is no problem and it is quite fast because it says simple approach. And the equilibrium calculation is quite simple. And you can have a table to be ready. It does not take into account the radiative heat loss. But it is infinitely fast chemistry assumption and equal the diffusivities.

So, the conditions which one can relax is that you can introduce more than one mixture fraction. So, this can be applied to more than one mixture fraction if you define. So right now, instead of that, if we say  $Z_1$  and  $Z_2$ , then we can easily solve three stream problem where first two stream will interact with  $Z_1$ , second stream will interact with  $Z_2$  and total  $Z_2$  function of  $Z_1$  and  $Z_2$  like that. Now we can add also in enthalpy in this in enthalpy deficit rather as an independent variable.

So that will take care of this radiation issues and all these things. And we can generalize this. Now when you look at this flamelet equation, what do we do? That is the step 1, how we go about it step by step process. Now, we have transport equation and the transport equations are defined in this  $x_1$ ,  $x_2$  and  $x_3$  coordinate system, this is our global coordinate system. Now, what is that a change of independent variable is made, which is like that the Z which is a function of these and we make it to other coordinate.

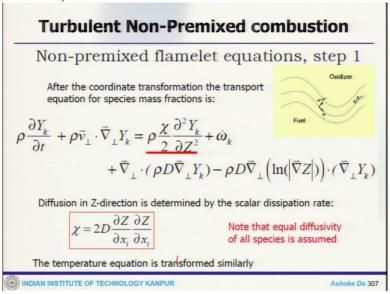




So, if we look at the flame front, this is the fuel, this is oxidizer and this is Z stoichiometric. So, in the flame normal direction there are local coordinate system one can define like this and this. So the local coordinate system with the first axis orthogonal to the flame front, increasing Z and the other coordinate orthogonal to the first. So, this is how with the increasing Z, we can see that because Z is sort of 0 here, Z is 1 there.

So, this is the 2 coordinate system that we defined. So, that means we have a global or Eulerian coordinate system from there we go to this local coordinate system in the flame front and that is why we keep on emphasizing this one is the prime normal kind of analysis, that means there is a transformation which takes place. Now, this is the coordinate system or they would say local coordinate system which is been defined along the flame surface or now we transform the species mass fraction equation.





So, the unsteady term will be there. Then this is the velocity in that local transport coordinate system, delta in the local coordinate system, there will be a term which is the diffusion of the species in jet with respect to Z that means, along these how these guy is actually baring. So, what can think about it instead of looking at the mass fraction equation in different three coordinate system now, we are trying to write the mass fraction equation in a single coordinate system of this, then reaction source term and we will get the other extra term like these, these and these.

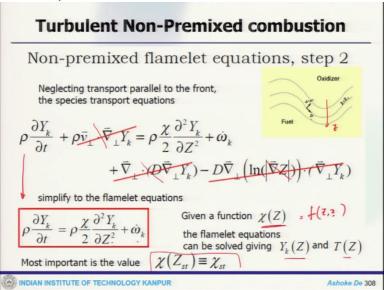
So, diffusion in the Z-direction can be determined by the scalar dissipation rate. So, this is how we define:

$$\chi = 2D \frac{\partial Z}{\partial x_i} \frac{\partial Z}{\partial x_i}$$

So, this is a connection if you see this is the term which actually a function of spatial coordinate of the physical coordinate which connects this transformation equation with this Z coordinate system or the local flamelet coordinate, but here one important thing that the equal mass diffusivity is assumed. So, similarly, one can transform the temperature equation to that means,

from this system to other system, so we get mass fraction equation, we get temperature equation which are transformed to so now they are in Z and time.

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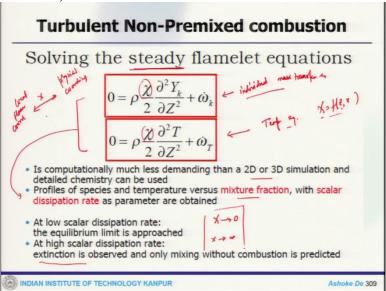


Now in the step 2, so we neglect some terms, so, neglect the terms which is parallel to the front in this species transport equation. So, if these are parallel to the front, these term cross out these term also goes off and this term also goes off. And what we end up getting it the unsteady terms of the mass fraction and diffusion term and the source term chemical source term. And here scalar dissipation rate guy becomes a function of Z.

Or rather it is a function of Z and local or I mean global coordinate system or the coordinate system with the mean flow field are solved. Now the flamelet equations which one can be solved, which is a function of Z and these for important value of scalar dissipation rate at stoichiometry. So, that is what you get that means, you see this is what after transform, this is what we get that means, our species mass fraction equation.

And temperature equation these are transformed to the local coordinate system or Z coordinate system or function of the Z. So these transformation that is why it is along the flame normal equation. This particular analysis is known as flame normal analysis.

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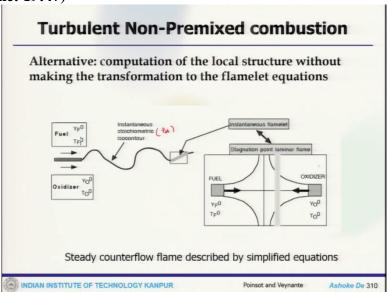
Now, you get 2 set of equation. One is for individual mass transfer equation and second is the temperature equation. Okay. So, both of them now, this is for a steady case and if you see that unsteady term is gone. Now, here, this is the term the scalar dissipation rate, which is a function of Z and local coordinate and spatial coordinate system of the global coordinate system. So, there is a connection between our flame rate equation and the flame normal coordinate system information with the global physical coordinate system information.

Because Z is also evolving in the physical coordinate system and scalar dissipation is calculated from there. And that is scalar dissipation rate is connection between or so, this is what you can think about the local flame coordinate to connected to the scalar dissipation the physical coordinate system. Okay. So, this connection is important what it is doing. So, if I look from the computational point of view, this is less demanding than 2D or 3D simulation and detailed chemistry one can use.

This is well solving the mass transfer equation one can incorporate the little chemistry and the reaction it has to be calculated. But importantly this is not done on the fly of the calculation. So, this is done in the pre-processing state. That means, these calculations are apparently done and then the lookup table has been created which is stored there and the information is faced out from there. Now, profiles of species and temperature versus mixture fraction and scalar dissipation rate as a parameter which are obtain by solving this set of equation.

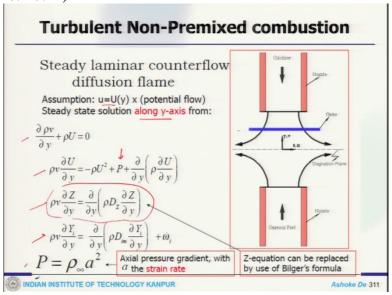
Now in the scalar dissipation rate is low that means it tends to zero which means the equilibrium limit is approached. If this is high then one can expect to have extinction and there will be only mixing without any combustion. So, there are two different limit of scalar dissipation rate.





Now, alternatively, one can have a calculation of the local structure without making the transformation of the flamelet equation. And how can that be done. You have a fuel and oxidizer and this is how the reaction flame front would be where the  $Z_s$ . This is Z stoichiometric line. And if you look at the situation where the instant in his flame front. And you can assume fuel and oxidizer are actually coming from the opposite side that means a counter flow configuration where you can get the stagnation point laminar flame and that may be used here.

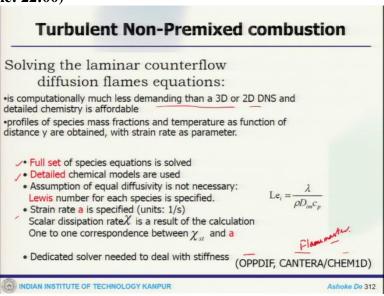
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Now, this steady laminar counter flow diffusion flame. Here this is our oxidizer. This is how fuel is coming. This is the coordinate system x and y and this is where the flame is sitting there and this is the stagnation flame. Now, the assumption is that u is function of Y and steady state solution along y axis. So, to get this equation then we get mixture fraction equation and species mass fraction equation.

Now, these particular one can that mixture fraction equation can be replaced by the Bilger's formula. So, that is one possibility of looking at it that one can do that. And secondly, the pressure can be correlated with the strain and the density. So, this is the actual pressure which is sitting there can be obtained. So, without transforming the system, we can actually write down the system in this fashion.

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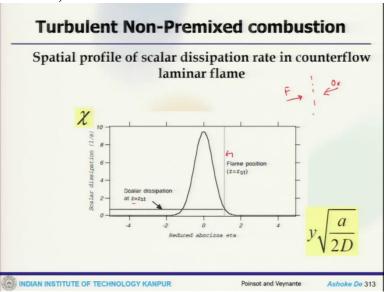


Now, you can solve this counter flow diffusion flame equations. This is computationally much less demanding than a 3D or 2D DNS or detailed chemistry. Now the profiles of species mass fractions and temperature as a function of distance y these are obtained and what it does, it solves the full set of species equations, which are solved, detailed chemical models are also used.

So, that means, detailed kinetics and all these things can be invoked and then Lewis number 1 or equal diffusivity is not necessary, strain rate is specified and scalar dissipation rate is calculated as a part of the calculation results. Dedicated solver who actually does this kind of

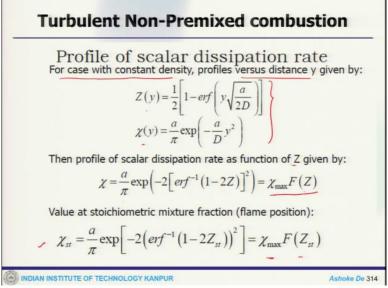
calculation like of the CANTERA, CHEMID or flame master something like that. So, these are the available one which one can use.

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Now, if you look at the spatial profile of scalar dissipation rate in the counter flow diffusion flame. So, this is the stoichiometric line and this is scalar dissipation rate, this is how it varies, this is the reduced y, and that is the position of the flame. And this is how this varies scalar distribution rate, so that give you an idea and this is fuel and oxidizer coming from opposite side. That is why it is called counter flow diffusion flame.

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Now, there are different profiles, which are available to represent the scalar dissipation rate. Let us say the case with constant density, profile versus distance is given as:

$$Z(y) = \frac{1}{2} \left[ 1 - erf\left(y\sqrt{\frac{a}{2D}}\right) \right]$$

And scalar dissipation rate is:

$$\chi(y) = \frac{a}{\pi} exp\left(-\frac{a}{D}y^2\right)$$

So, this is for a constant density situation and the profile for scalar dissipation rate as a function of mixture fraction was given as:

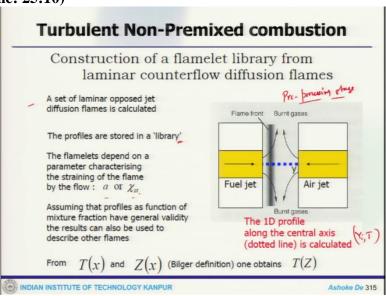
$$\chi = -\frac{a}{\pi} exp(-2[erf^{-1}(1-2Z)]^2) = \chi_{max} F(Z)$$

And similarly, you can find out the stoichiometric scalar distribution rate which is:

$$\chi_{st} = \frac{a}{\pi} exp(-2[erf^{-1}(1 - 2Z_{st})]^2) = \chi_{max}F(Z_{st})$$

So, this is what one can get for different profiles.

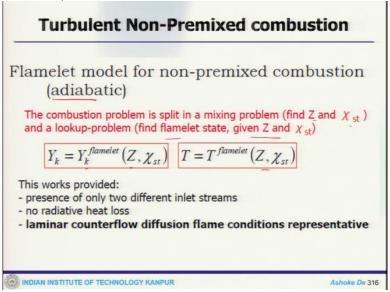
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Now, you can look at the construction of a flamelet library from laminar counter flow diffusion flames. You have a fuel jet coming in here and this is what the burnt gas so after that it is all one new profile along the central axis and where you can see the various end of the species mass fraction temperature and all these. So, you set up laminar opposed diffusion flames, a calculated and then the profiles are stored in a library. So, that is important that is why I said these things are done at the pre-processing stage.

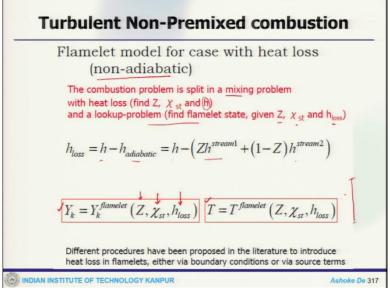
So, it is not what usually takes place during the calculation and then it depends on the characteristics straining of the flame that a or  $\chi_{st}$  and then we assume the profile for T and Z.

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So, now if you see the flamelet model for non-premixed combustion which is an adiabatic one that means there is no heat loss. So, the problem essentially split into 2 problem 1 is mixing problem, finding Z and then the  $\chi_{st}$  and then look up problem that means, the flamelet state were given Z and  $\chi_{st}$ . So, we have species mass fraction and mass fraction when it is a flamelet there is a function of  $\chi_{st}$  and when there is a temperature, then lead temperature and this. So, this works nicely for 2 stream and also it does not take into account radiator heat loss and these are some sort of representative situation now.

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Another case could be where you have heat loss that means a non-adiabatic situation. So, the problem definition still remains same that means, you still split into two problem, one is mixing problem and another is the heat loss problem. So, that means, now you have to take into account

one more extra variable that is the enthalpy. I mean usually people take into account the enthalpy deficit or something like that. And then you lookup the table based on Z stoichiometric and heat loss.

Now, heat loss what is the enthalpy and adiabatic one. So, it will be each  $Zh^{stream1}$ ,  $Z^{stream2}$  and then your species mass fraction and temperature they will become a function of Z which is evolving in the spatial coordinate system or the global coordinate system,  $\chi_{st}$  which is a function of the Z and that is also dependent on the spatial and the heat loss. So, once we get this then you can actually estimate your mean profile using the assumed pdf.

Now, different procedures are there or have been proposed literature to introduce this flamelets and considering the heat loss and all this, I mean these are again what we are doing here discussion is the basic of all these things, but one has to look at the current literature where there are plenty of advancements has been made because these things were proposed long time back and after done it has been modified.

So, one can think about these as quite standard methodology or approach for calculating the turbulent non-premixed flame and there is a huge literature database which is available and one can see how people come up with a different ways to different multi stream problem and etc. So we will stop it here today and continue this discussion in the next lecture.