Turbulent Combustion: Theory and Modelling
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Lecture - 56
Turbulence-Chemistry Interaction (Contd...)

Welcome back. So let us continue the discussion of turbulent equation for non-premixed combustion, we have looked at the adiabatic system and non-adiabatic system. Now we are looking at how we can model this turbulent equation. So, we had looked this non-adiabatic system and adiabatic system.

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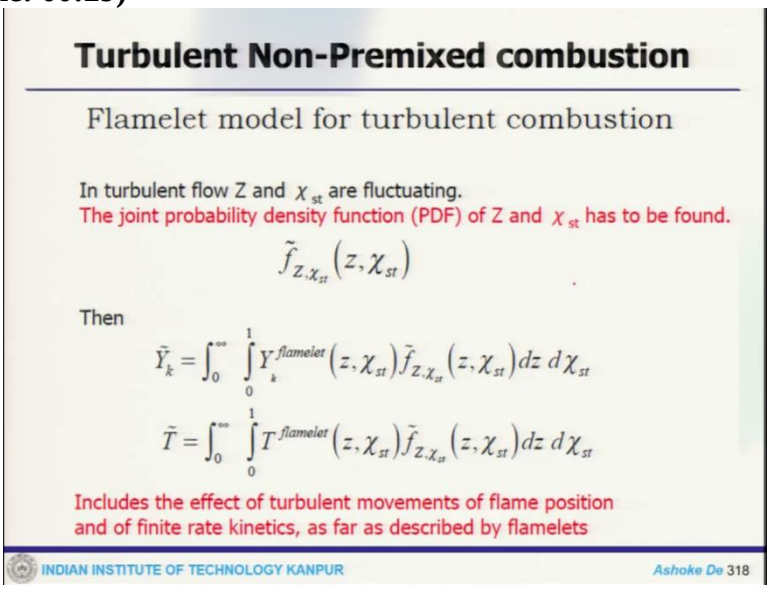

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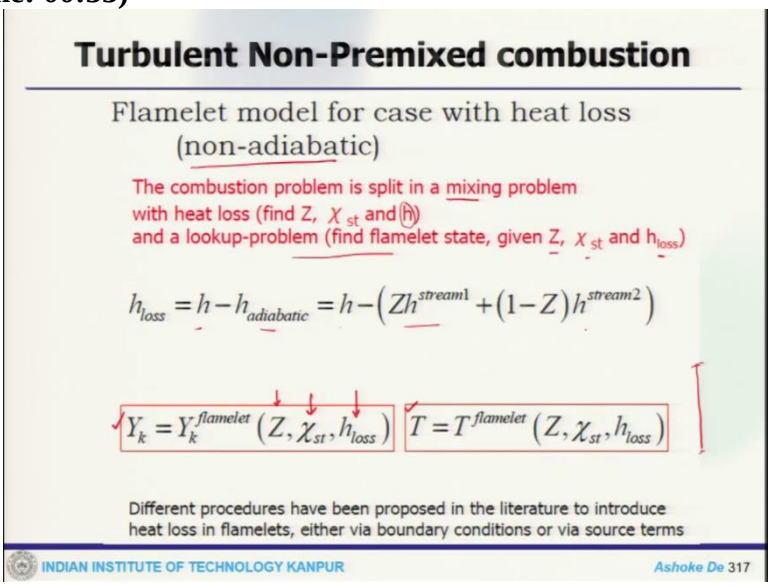

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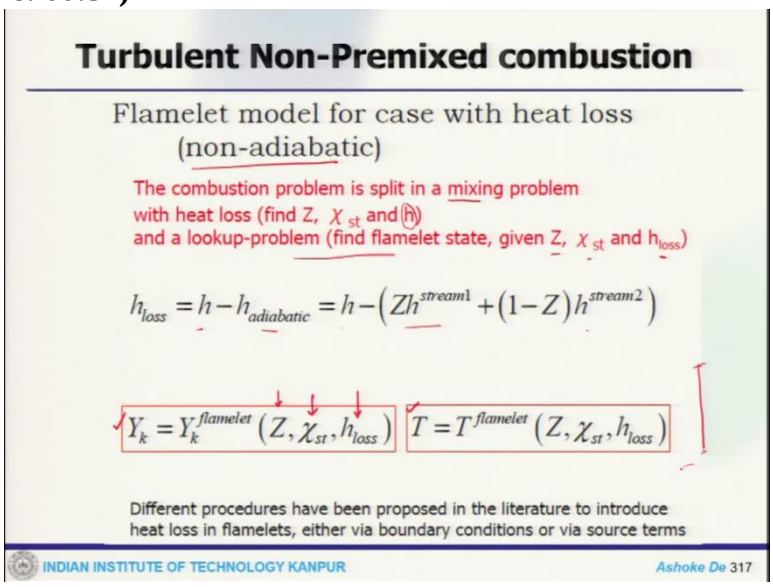

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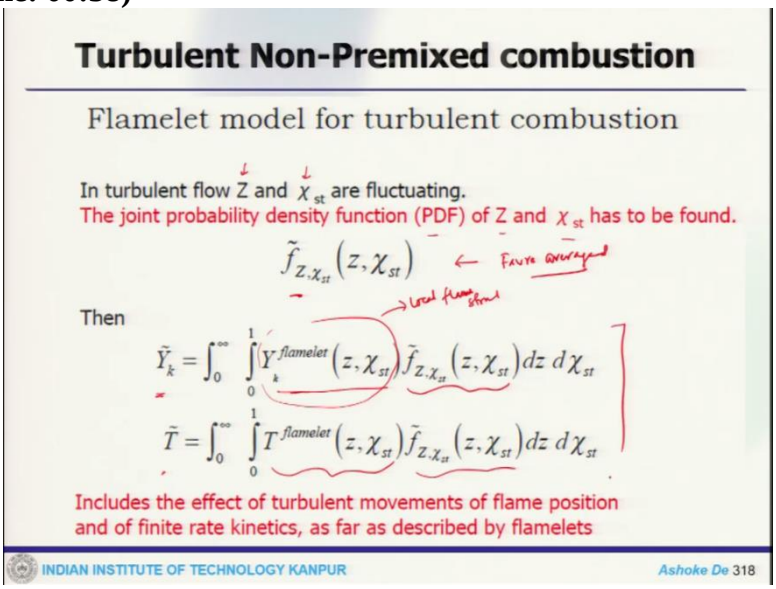

And now look at when you have this turbulent combustion, mixture fraction and stoichiometric scalar distribution rate, they are fluctuating. So, you need to define this PDF or quality density function of Z and χ_{st}. So, once you define that this has to be found that means the joint probability density function, this is again the Favre average terminology. So, then you can find out your means which is mass fraction using 0 to 1 and 0 to infinity. This is mass fraction variable, which is a local flame structure this is all local flame structure and the probability density function. Similarly, mean temperature one can find out is in the local variable of the T and the PDF function. So, this includes the effect of turbulent movement, flame position finite rate of kinetics everything. So that is how you obtain from there.

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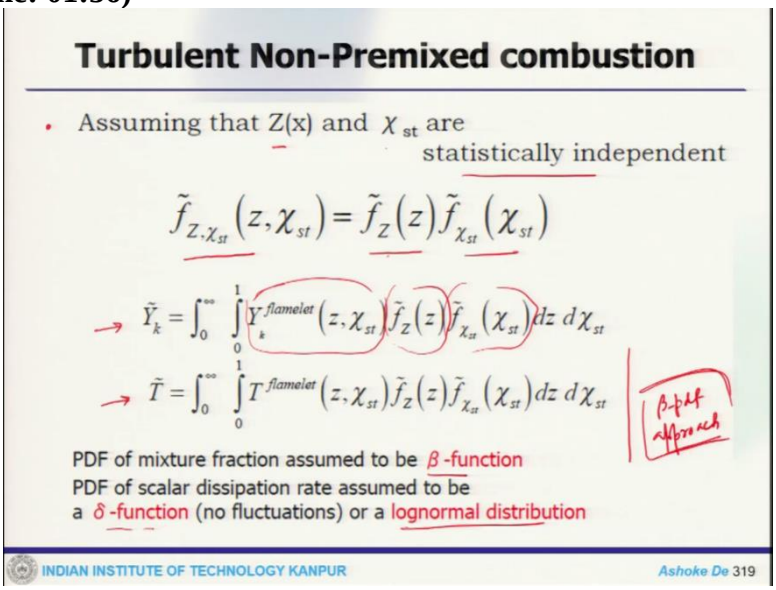

Now, if we assume this is again a specific case where you assume that Z and χ_{st} are statistically independent. If it is statistically independent what we have already seen in statistical description of the turbulence this joint PDF function which is a function of z, we can write in individual function like this. If Z and χ_{st} in that case, what will happen that this calculation of the mean mass fraction or calculation of the mean temperature can be modified.

This is again local flame structure and this is the density function for mixture fraction. This is the PDF function for the stoichiometric scalar distribution rate. So, PDF mixture fraction assumed to be a beta function and PDF of scalar dispersion rate assumed to be a delta function, no fluctuation, it is a long normal distribution. And sometimes that is why literature you can see this presume PDF approach is also called the beta PDF approach.

This is another terminology which you may come across while looking at this thing, because that is how you assume the shape of the PDF to find out the mean profile.

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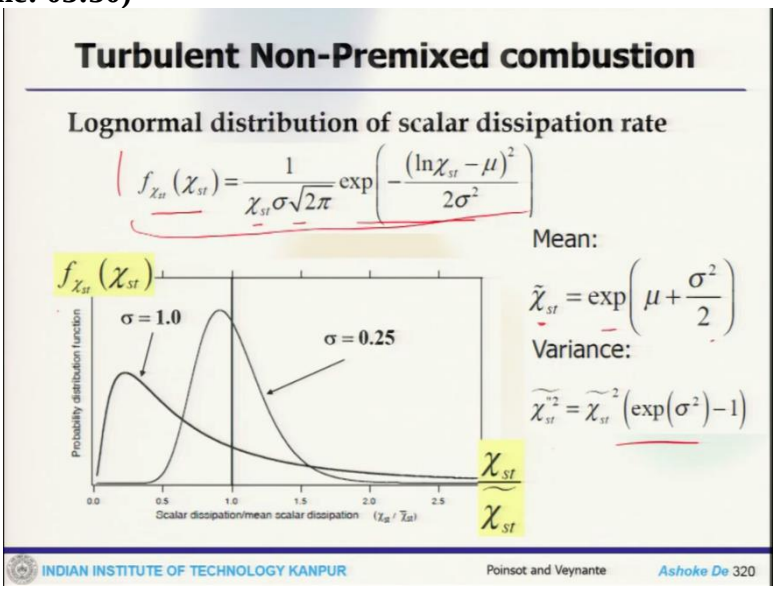

Now, for the scalar dissipation rate, if you look at the normal profile or normal distribution, log normal distribution, this is how the probability density function PDF of the stoichiometric scalar distribution rate which is written is:

$$f_{\chi_{st}}(\chi_{st}) = \frac{1}{\chi_{st}\sigma\sqrt{2\pi}} exp\left[-\frac{(ln\chi_{st}-\mu)^2}{2\sigma^2}\right]$$

Now here, the mean of scalar dissipation rate and it would be:

$$\tilde{\chi}_{st} = exp\left(\mu + \frac{\sigma^2}{2}\right)$$

And the variance would be exponential like that. Now, if you look at the plot these direction of scalar PDF of the stoichiometric scalar distribution rate and these direction we are plotting the stoichiometric versus the mean it is an shorter than ratio and for different variance sigma 1 sigma 2.5 we will see how this log normal distribution varies. So, this is an already assumed function that means I know the quality distribution function which is advantageous compared to solving the individual PDF transport equation which is quite expensive in nature.

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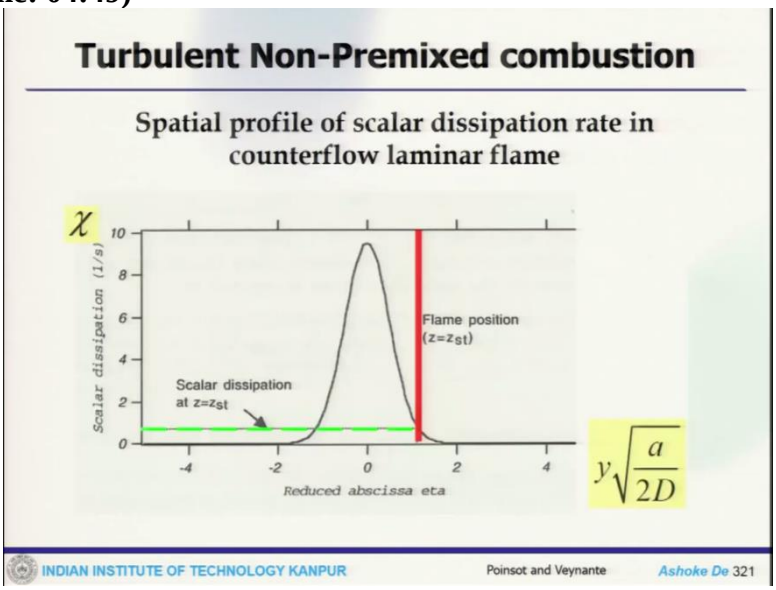

So, that is another aspect of how. Now if you look at the spatial profile of the scalar dissipation rate in counter flow laminar flame, this is how long the rate and this is the reduced coordinate this is how it moves this already we have seen there is nothing like that.

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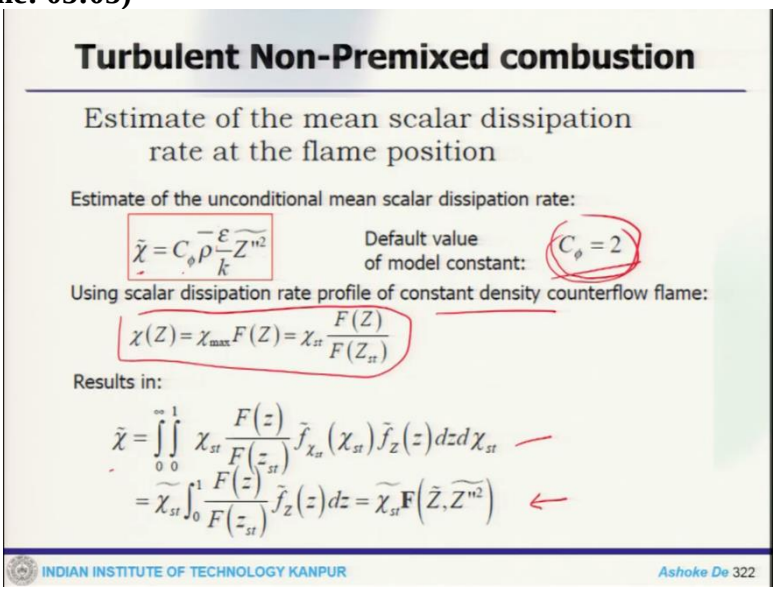

Now, the point which is quite important is that how we estimate them mean scalar dissipation rate at the flame position. So, we estimate the unconditional mean of scalar distribution rate, which is like this, which can be estimated like:

$$\tilde{\chi} = C_\phi \bar{\rho} \frac{\varepsilon}{k} \widetilde{Z''^2}$$

Now, C_ϕ is a model constant and typically value of 2 is used. Now, this is essentially a constant which takes into account the ratio of the timescale between flow and kinetics. And here is the

timescale of the turbulence structure $\frac{\varepsilon}{k}$. So that is why large or wide range of problem this model constant of C_ϕ equals 2 works nicely. But when you go to some specific cases like hot flow conditions and all these were auto ignition, I mean, is the primary dominant mechanism that time or rather where the frame is kinetically control rather than the mixing control this value may not work one has to tune it.

Now, if you look at the scalar dissipation rate profile at constant density, this is how one can represent this and this will get you the mean scalar dissipation rate in terms of 0 to 1 like this, and you can do the simplification and get like that. So essentially if I put these things together.

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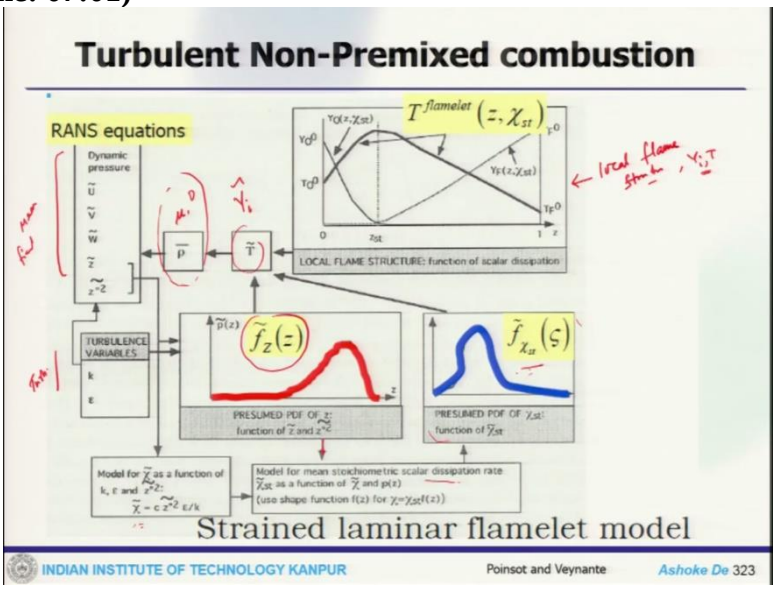

That is how you have it from your completely strained laminar flamelet model and how it works. So, you solved the main flow field along with turbulent equation, this is our mean field and this is a flamelet approach, I mean, one information which is required is the local flame structure, this is our local flame structure. So, all your species mass production, temperature. These are solved using digital kinetics and the values are stored. Now, first thing what happens is that using the information of mixture fractions and its variance and also the information of the turbulence, we first fit in there, and we get the probability distribution function of the Z. This is the probability distribution function and that we have seen how we can obtain that is essentially a gamma function and using the Z and Z variance, you can do that.

Now, we have also presumed probability distribution function from the χ, which is a log normal distribution. Now I feed the information of Z and Z variance here, and model χ as a function

of k, ε and $\widetilde{Z''^2}$ which is χ is $C_\phi \frac{\varepsilon}{k}\widetilde{Z''^2}$. Now, we can model for mean stoichiometric scalar distribution rate, which is a function of Z and the Z function. So using these distribution function and also the information of mean scalar distribution rate, we find out this. So, which will give me this presumed PDF of the χ T. It was typically the log normal distribution. So, that means, when you looked at the equilibrium set of calculations, this portion was not there, we had a distribution function of Z, local flame structure from the equilibrium and they used to get it now.

Here you get Z and Z variance using that you calculate χ, the scalar dissipation rate χ to stoichiometric scalar distribution rate mean and then finally the distribution function. So, this one and this one together with the local flame structure get mean temperature profile or Y and Y_i all these. And then finally, you get ρ and viscosity if it is temperature dependent, these will be fed to the main profile that means again these are the properties like density, transport properties. They are sent back to the main flow field and main flow field is actually taking those things into account and it is all for the main flow field. So, this is how the mixture fraction based situation actually works.

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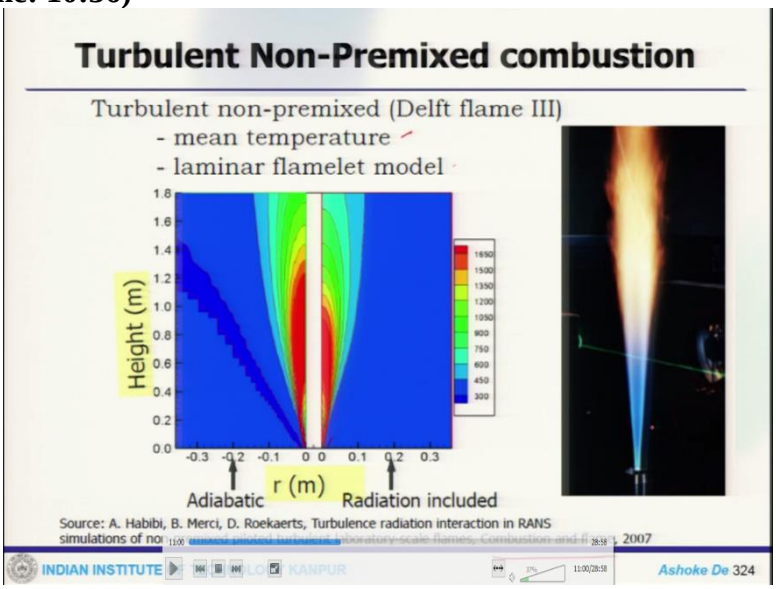

Now, if you look at some of these examples. So this is taken from this literature is the natural gas flame, here is the mean temperature profile and laminar flamelet model for you can see the predictions how it is obtained? This is the flame structure.

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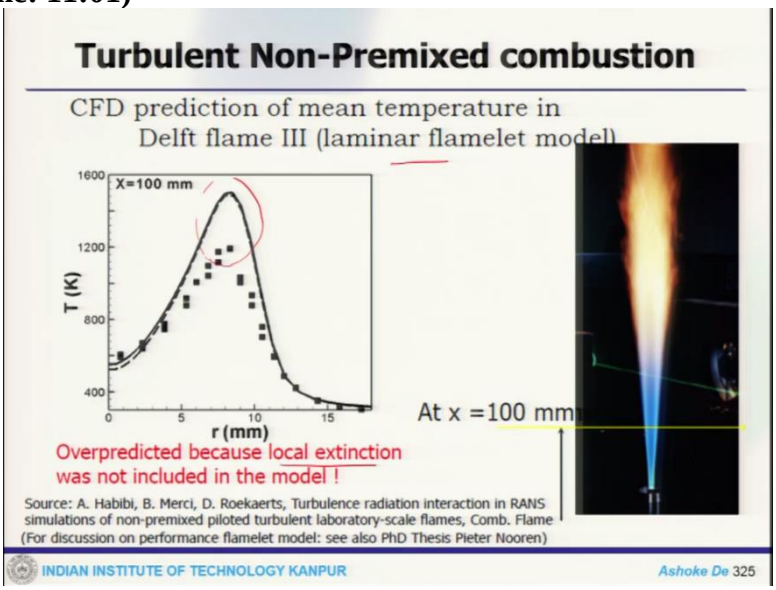

So, now this is another for the same using this flamelet model, how we get the radial distribution of the temperature of these things. So, there are some over predictions of the local extension because these temperature profile is over predicted as the flamelet model does not take into account the local extinction. Okay. So, this is what give you an idea if you look at this literature, this will give you an idea of the different issues of flamelet model and all these things.

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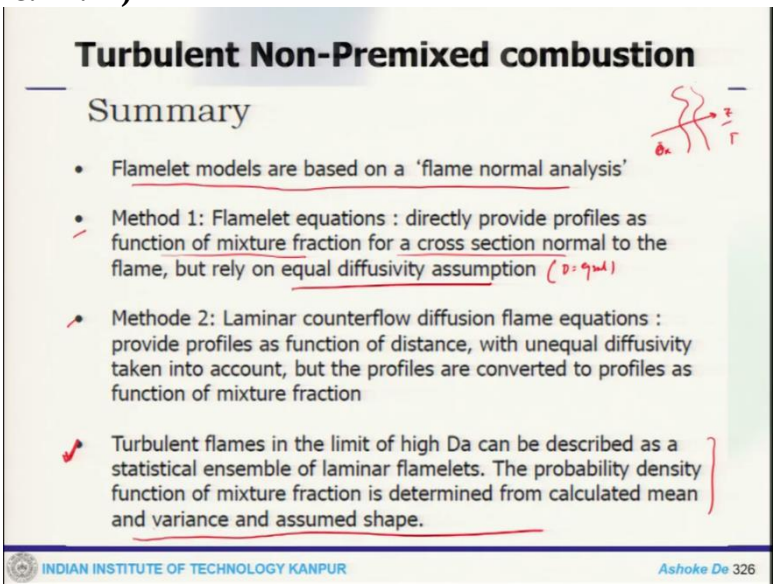

So, that is pretty much what you have in the flamelet zone, and if we put them what we have discussed. So, what is that? Flamelet models are based on completely flame normal analysis which is absolutely important because that's where if you have a local flame structure like this along the normal direction we do the calculation. Now, flamelet equations which are provided the profiles as a function of mixture fraction for a cross section normal to the flame.

But they rely on the equal diffusivity assumption. This is an important assumption. Now, third the laminar counter flow diffusion flame equation which can provide the function of distance profiles which are converted as a profile of mixture fraction. Now, the important is the turbulent flames in the limit of high Damkohler number can be described as a statistical ensemble of laminar flamelets. The probability density function of mixture fraction is determined from calculated mean and variance and assumed shape.

So, this is what it is done to estimate the realistic situation. So, that is pretty much what or how you get to the laminar mean flamelet kind of system for the non-premixed case. Now, we can look at some comparison of these flamelet model and the PDF model.

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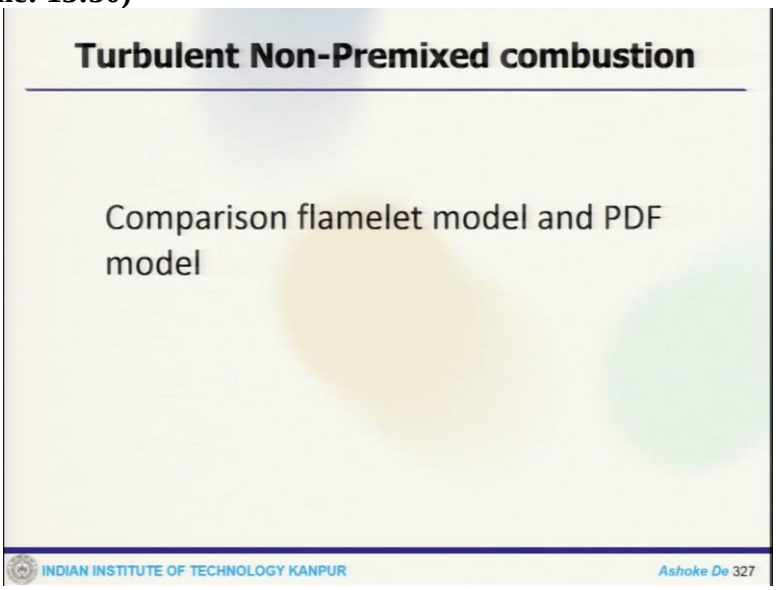

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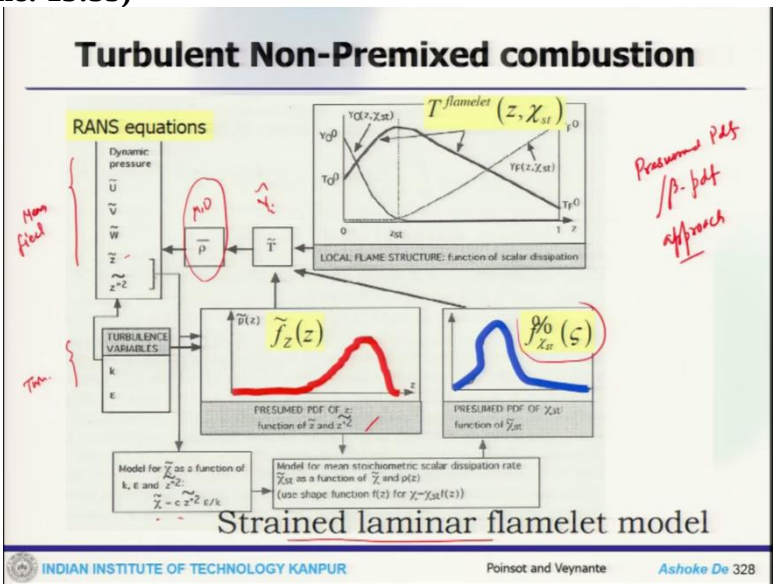

And that will give you what we have discussed under this non-premixed combustion, everything will be qualitative and it will give you a quick refresh of the whole thing that we have talked. First look at the strained laminar flamelet model. Another name is the presumed PDF or beta PDF approach. Okay. You have a RANS equation where mean field are solved. Then we have turbulence equation for the turbulence informations are coming into the picture in the meaningful profile equation which are mixture fraction on and is variance. So, using that we get it using that turbulence information also we get scalar dissipation rate which is estimated like that means scalar dissipation rate we get stoichiometric scalar dissipation rate which will lead to this presume safety of the quality distribution function of that.

And then same thing using the mixed fraction and variance. We get the presume shape of the PDF for the Z and these 2 PDF along with the local flame structure which is apparently calculated, we get all the mean profile. And then finally, all these transport property, which are sent back to the mean flow equation to make the handshaking. So that is what we do. One thing it is very fast competition list demanding and can be applied to a large scale of problems.

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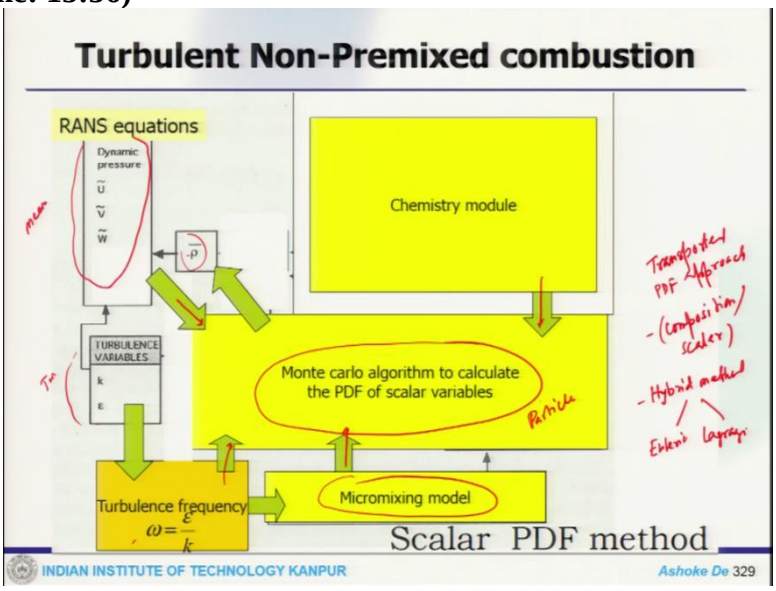

Now, this is scalar PDF equation that means or it is in transported PDF approach. They are under that it is a PDF composition or scalar PDF. Here we solve the transport equation for the probability density function or probability distribution function. And this is where it is computationally expensive procedures we adopt hybrid method. So that hybrid method is we solve both Eulerian and Lagrangian. So, this is where we solve the mean flow field we solve turbulent also. So, these are turbulent mean flow field calculation. So, the turbulence equation using that we get that turbulence frequency, turbulence frequency goes to estimate the micro

mixing model and the same time mean flow field information passed turbulent frequencies passed micro mixing model using that we solved the Lagrangian equations in the Monte Carlo system.

Where these are input turbulent frequency input, mean flow field information, mixing model, reaction model everything is so, there we solve individual particles or this is solved in the particle approach. So, particle position their mixing reaction, mixing and all these things are taken into account. From here we estimate again density and other transport properties like viscosity and all these things which are sent back to the meaningful real equation. That means, if you look at it the commonality between these approaches with a transport PDF approach or the presumed PDF approach, the mean density or other transport properties which are coming out to be the parameters they do the making that bridging between the mean flow field and the local situation.

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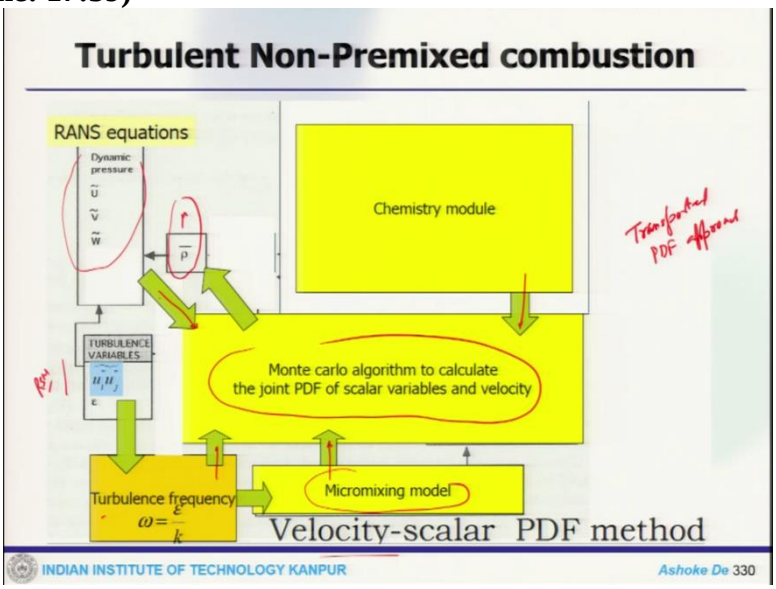

This is again transported PDF approach. But this is now velocity scalar composition PDF that means you require joint pdf and all these things. So, idea is similar you solve the mean flow field here you solved specially RANS kind of equations or you have individual unique system which are solved and also the dissipation which are solved and using that you get turbulent frequency. And that is passed for the micro mixing model and that information is feed frequencies is feed, mean flow field information kinetics comes here then the lagrangian solutions are obtained in the Monte Carlo technique and using that finally, again the density, viscosity these are the parameters or which will be fed to the mean flow field equation and we solve for that.

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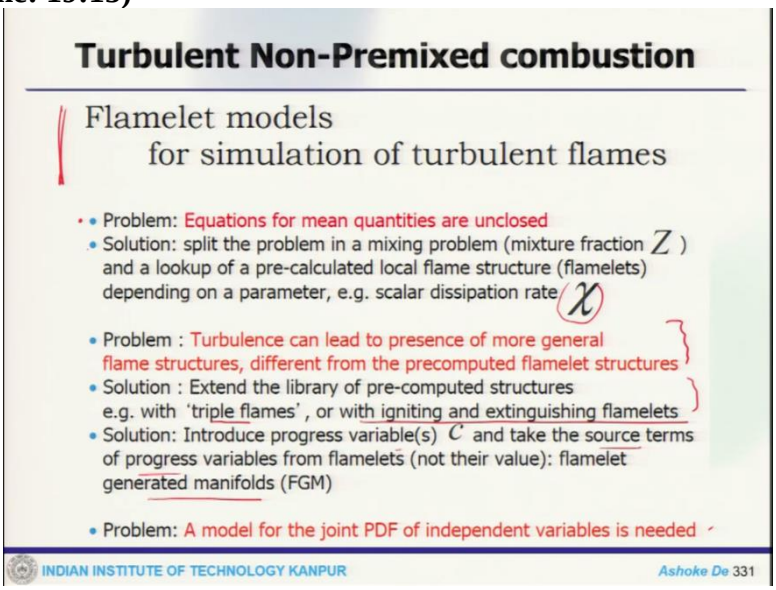

Now, if we look at this flamelet models and that issues, the problem here, equation for the main quantities are unclosed. So that is why the problem is split into 2 problems. One is the mixing problem, which is the mixture fraction and a lookup table which is calculated or pre calculated using the local flame structure known as flamelet, depending on a parameter of scalar dissipation rate χ.

Now, this is one of the problems which are handled in this way and that is why make this process to be generic enough for the second problem which is there is a turbulence can lead to presence of more general flame structures, different from the pre-computed flamelet structures or one way to solve this problem, extend the library for pre-computed structure with triple flames or with the igniting and extinguishing flamelets. So, that will allow to at least go to certain limits.

Or alternatively, one can introduce another scalar transport equation in terms of a flamelets a progressive variable and take the source terms of progress variable from flamelet. And this is going to be FGM kind of approach that is the flamelet generated manifold kind of approach. So, that means, not only depending on the local value of mixture fraction and variance, also, you solve for the progress variable and now using those information you can actually sort of handle this kind of problem.

My model for joint pdf or independent variable is needed, this is another issue that one has and these are the some of the problems one can think about by looking at.

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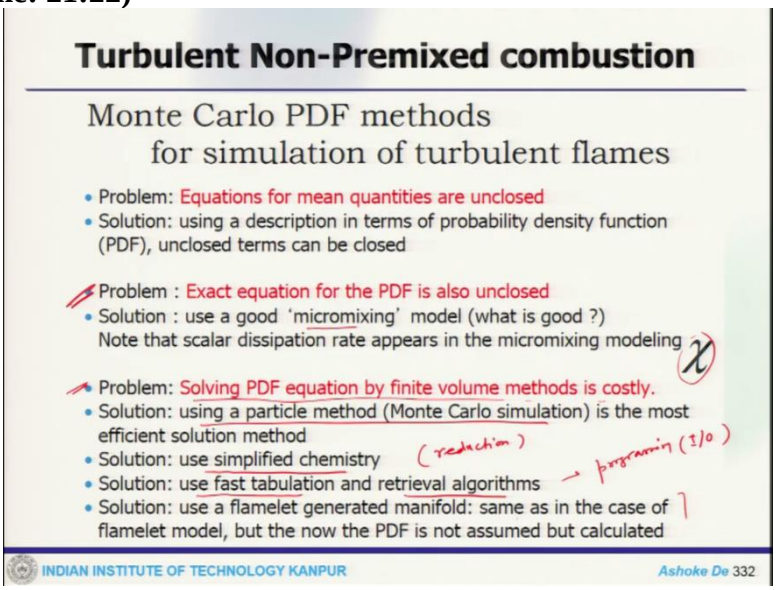

Similarly, if you go to the transported PDF approach or Monte Carlo based PDF method, so, one problem equation of the main quantities are unclosed obviously, but the chemical system remains closed. So, using the description of the probability density function, that source terms and other terms are closed. Also, another problem which comes in is this problem that the exact equation for the PDF is also unclosed.

So, we use some approaches and for that and using the mixing model to close that term and the scalar dissipation rate, which is the χ that appears in the mixing model, but now the mixing model or the accuracy of the mixing model or the fidelity of the mixing model can have a lot of impact on this thing in closing these terms. So, that is another point here, one has to look at what kind of mixing model.

Or what because, we have already seen 3 different kind of mixing models. Now, third problem is that solving PDF equation by finite volume kind of methods are quite expensive, which is true and that is why we go back to particle kind of situation or Monte Carlo kind of situation. So, that is one of the most efficient method to solve it. Then obviously, you do some trade off in the solution using some sort of a simplified chemistry.

That means, you do that reduction instead of using detailed chemistry because more and more chemistry if you used it would become uncomfortable really expensive. So, that is another then use some fast tabulation and retrieval algorithm. That means, the tabulations and the retrieval this is something to do the programming skill because one has to write the IO functions to be

efficient and optimized, then you can use a primary generated manifold same as in the case of flamelet model, but the PDF is not assumed but calculated.

So, now if you see this, this is all discussion on something which is related to the PDF kind of model that is you can have presumed PDF method.

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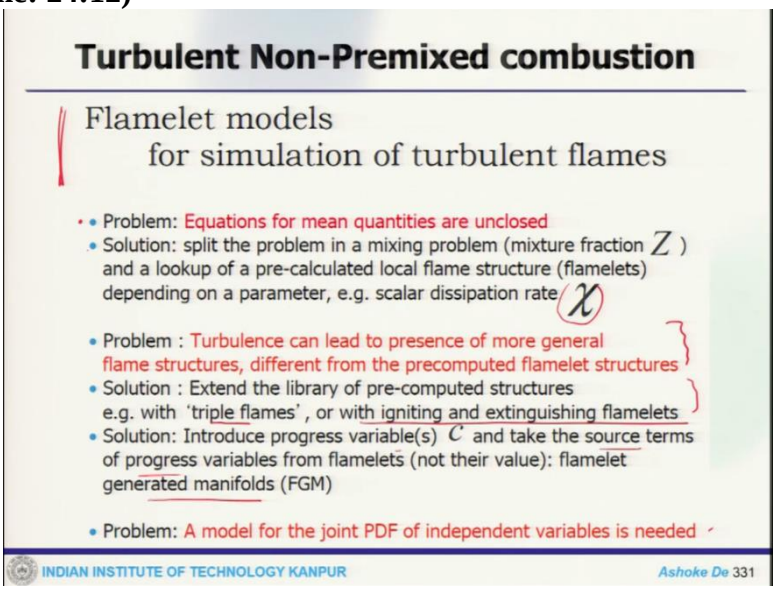

Or better PDF method where you it is competition less demanding, it is quite fast can be used for a wide range of non-premixed combustion models.

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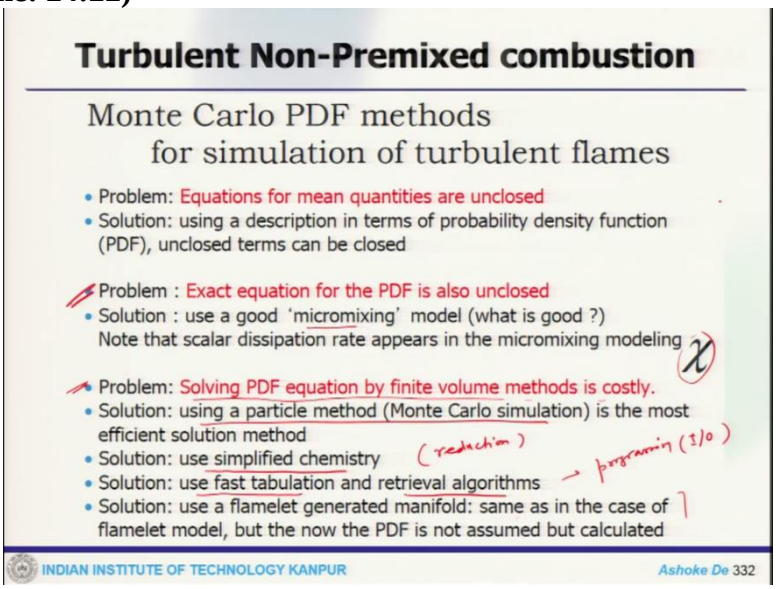

But when you look at the Monte Carlo method they are expensive. Obviously, you do not have to assume the PDF distribution apparently. So, it could be accurate and this provide reasonable

a good prediction for the non-premixed cases and premixed cases you require fine tuning, but theoretically this should be applied to any mode of commercial. So, that is what it is.

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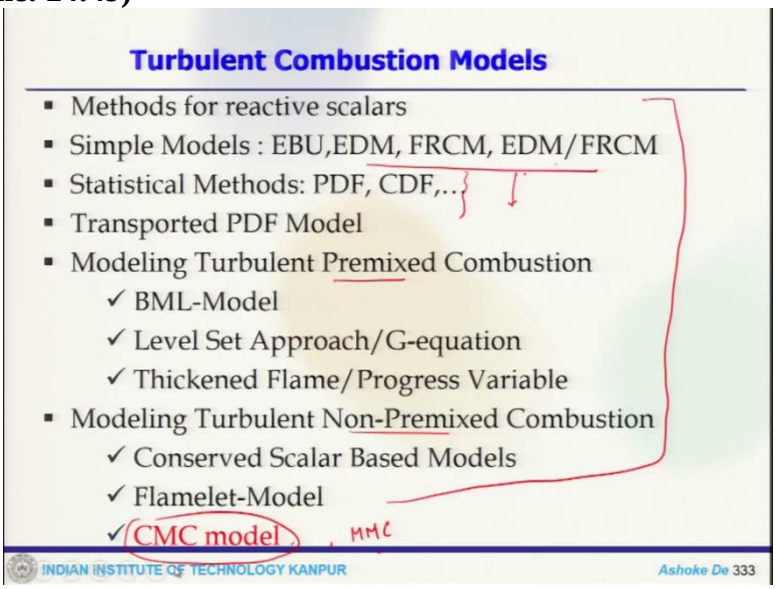

So, that is pretty much if you look at this chart, we have pretty much covered all the discussion except this last one which we are going to now do this is one of the advanced model. So, you have to refer to the literature and there is another advanced model which is called MMC models multi. So this CMC is conditional mapping closer and this is multiple mapping closer and will give you an idea, or we will do some discussion on CMC and MMC will do while talking about the multi-phase close little bit.

So, that will give you how we started with the simple reaction models, then issues that we have discussed then move to the statistical based model. Then finally, some models for premixed combustion, then we have looked at non-premixed. And now we are going to look at this CMC one.

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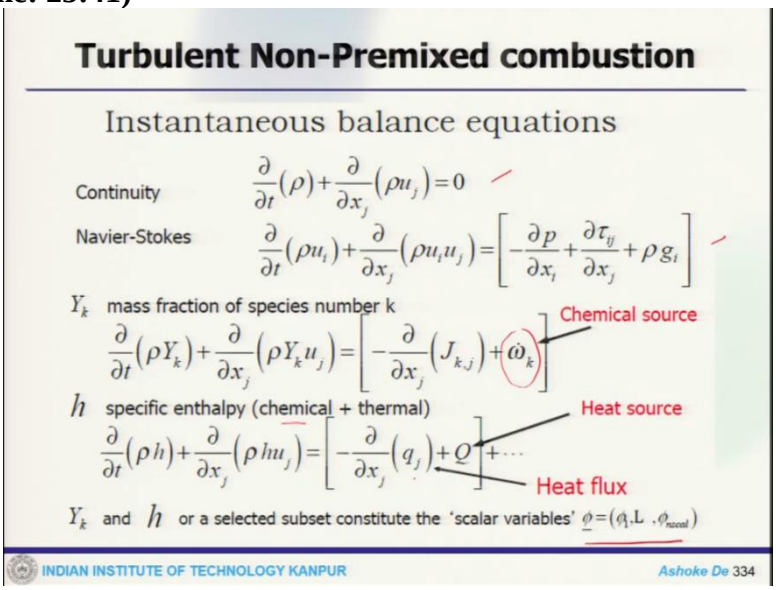

Now, here, the instantaneous balance equations, we have to start from that our basic set of equations, which are continuity, Navier-Stokes species mass fraction of species number system which we will get back and the enthalpy equation in the total enthalpy which is chemical and thermal. So you get heat flux, heat shows another term. So, if you put the scalar variable this would be the functional and it says set of scalar variable which will include all the mass fraction, add in enthalpy this.

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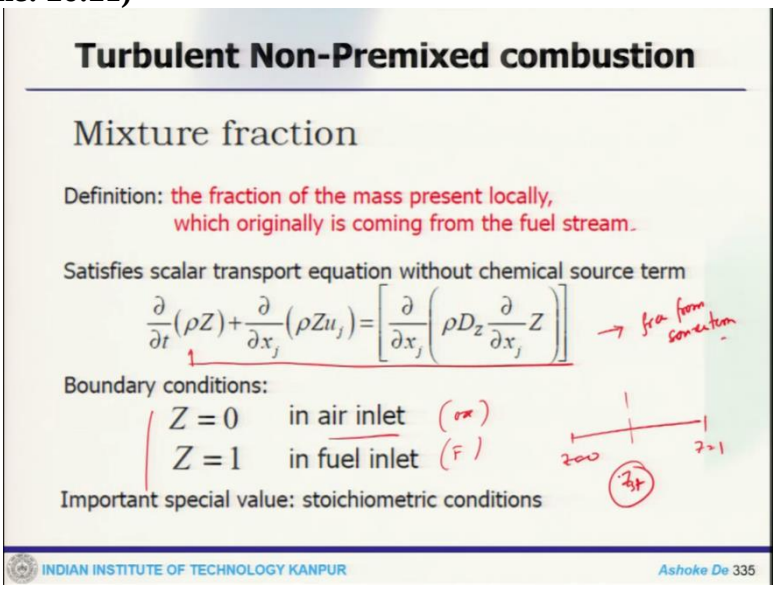

Now again, we need the definition of mixture fraction. So the fraction of the mass which is present locally, and we will get the mixture fraction transport equation. I mean this is again free from source term, I mean chemical source term that is a biggest advantage of that thing. And then, you put the boundary condition this is in the oxidizer inlet and this is fuel inlet. So

Z is 0 and 1 so they will vary between 0 to 1 and the reactions takes place along Z stoichiometric. Right?

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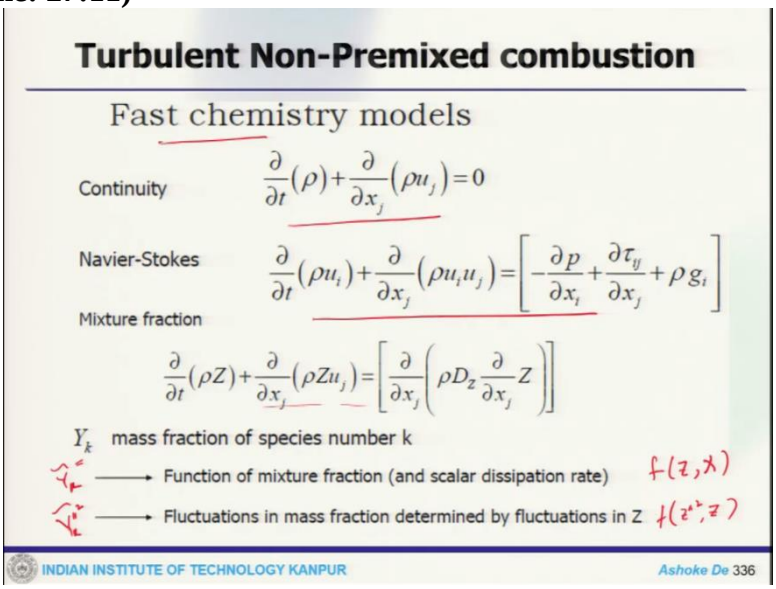

And if you have fast chemistry model, then you get this is the continuity, momentum and the mixture fraction equation. So, here Y_k will become a function of mixture fraction and scalar distribution rate and the fluctuation in mass fraction is the fluctuation in Z. So, that means, this is Y_k prime and this is Y_k. So, one and so this would be function of Z variance and obviously, Z has to be there.

So, you can take into account the function like this in the fast chemistry models and these are detailed discussion that we have done that. Now we can see the different relationship, but that will do in the next class. We will stop here today. Thank you.