Turbulent Combustion: Theory and Modelling
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Lecture-57
Turbulence-Chemistry Interaction (contd…)

Welcome back, let us continue the discussion on our non-premixing combustion and we are now going to discuss on the CMC model and all this. So, we have looked at different non-premixing combustion modeling approach like mixture fraction based approach, where you split the problem into different problems and then assuming the beta PDA, you can close the mean value of mixture mass fraction and the temperature.

And alternative was there the transported PDF approach and we have seen what are the issues associated with that and how usually we handle that. So, now we are last part of it. One of the advanced model is the CMC model. Again, this is quite specific to the application of non-premixed combustion.

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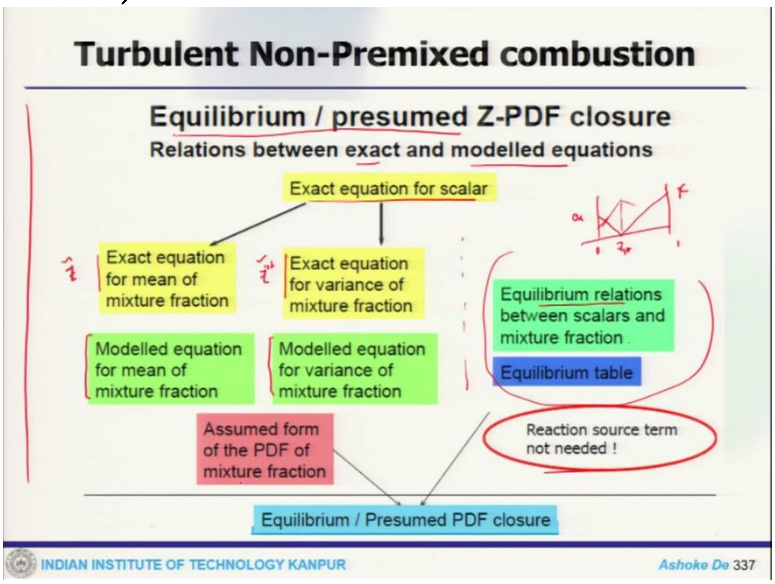

So, this is where we wanted to just to recap the whole business and then this will give you a relationship between our exact equation and the modelled equation. Now, this is our equilibrium or presumed Z-PDF closure. That means it is a PDF kind of approach, which is computationally less demanding. So, we have exact equations for scalar. This is what we get from there.

We get exact equation for mean and mixture fraction and from there also, we get the variance. That means, this is there and this equation is for variance. So, we get exact equation for that. Now, we get the modelled equation for mixture fraction model equation for the mixture fraction variance. Now, on the other side, this is one side of the whole thing. On the other side, you have equilibrium relations between scalar and mixture.

Fraction equilibrium table or it could be flamelet table and assume PDF from the PDF mixture fraction and then you do not have any reaction system here in the equilibrium table, the whole assumption is that as soon as things comes in contact, they actually burn and you get the temperature rise. So, this is a burning yet get stoichiometric. This is fuel and this is oxidizer. So, the equilibrium is in PDF cruiser. So, this will give you the complete picture of the whole process. And this portion is the local name structure, this is your mean variables and all this.

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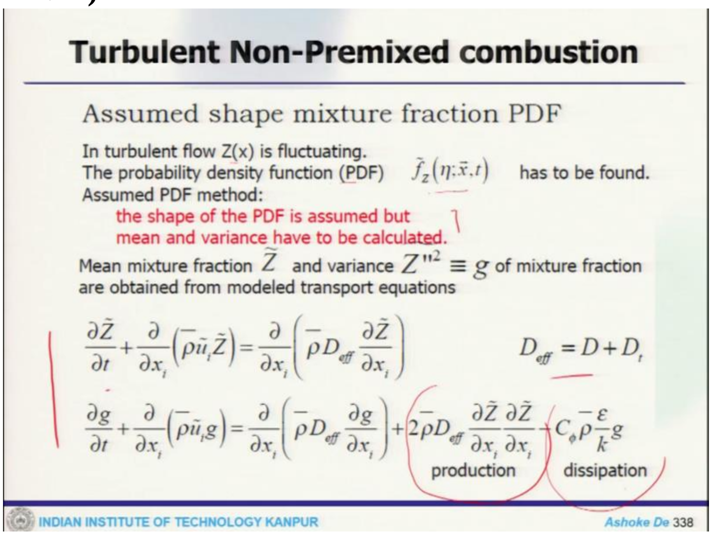

Similarly, if you have assumed shape mixture fraction PDF, we saw the Z(x) is fluctuating. So we need to have a problem density function which is to be found. So that shape of the PDF is assumed and mean and variance we are calculating. So we get 2 set of equation: mean and variance and the variance equation has the production term and dissipation term and this is all the effective diffusivity is estimated. So, once we do that, then see how the whole thing works actually.

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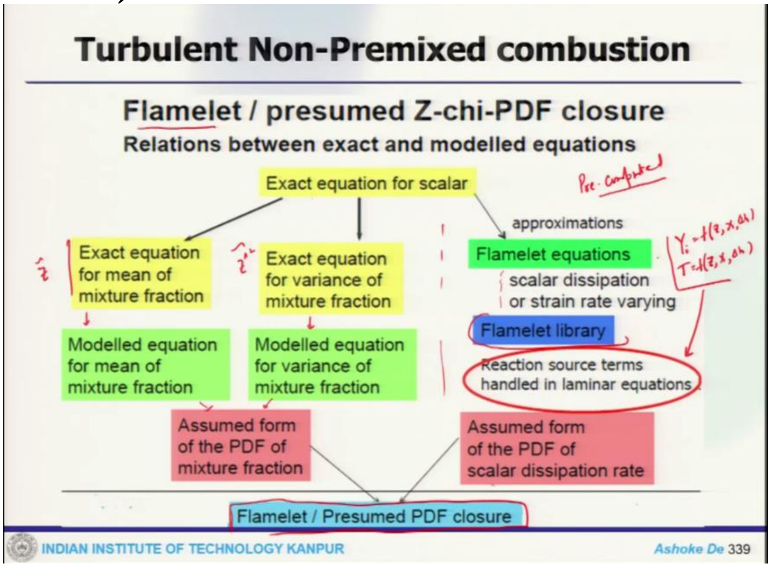

This is called flamelet equation or Z-chi-PDF closure. So, you have exact equation for scalar. So, we get mean we get variance and from there get the modelled equation, this is the model these things. Now, from the scalar we have flamelet equations where all our mass fraction becomes function of the scalar dissipation rate and possibly Δh the non-adiabatic system. Temperature is also a function of Z-chi and Δh.

So from there, using the scalar dissipation and or the varying strain rate, we get flamelet library. So, this portion is again pre-computed that means, this is not done on the fly this is done a priori and the calculation is told and then the reaction source time is handled in laminar equations that means, when we solve the set of equations, this actually takes care of the reaction source.

From here, we get the assumed form of the PDF of scalar dissipation rate. And here we get the assume shape of the PDF or mixture fraction using these 2. We will finally close the presumed shape PDF for this.

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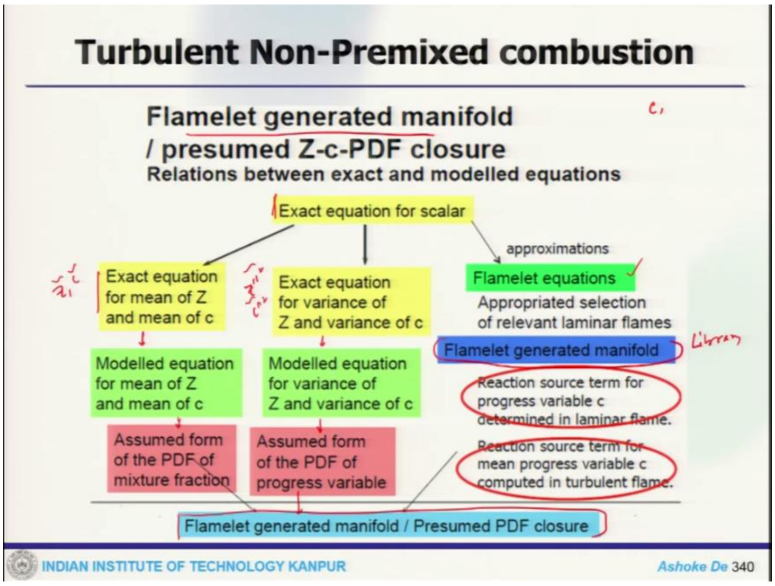

Now, another way is that, when you want to take into consideration the progress variable C So, We called is flamelet generated manifold or presume Z-c-PDF closure to we have exact equation for scalar. So, we have mean equation for Z and c. We have variance equation for Z and c and then we get the modelled equation from there. Now we have assumed PDF from the mixture fraction, we get another PDF for the progress variable also. And then another side, we solve the flamelet equation and from the flamelet equation, we calculate this library which is a function of here we have reaction source from for progress variable. And we have reaction source term for mean progress variable c on the turbulent flame. So, we have everything here which are included. Now using this table and these PDF shape, we get the flamelet generated manifold or presumed PDF these things.

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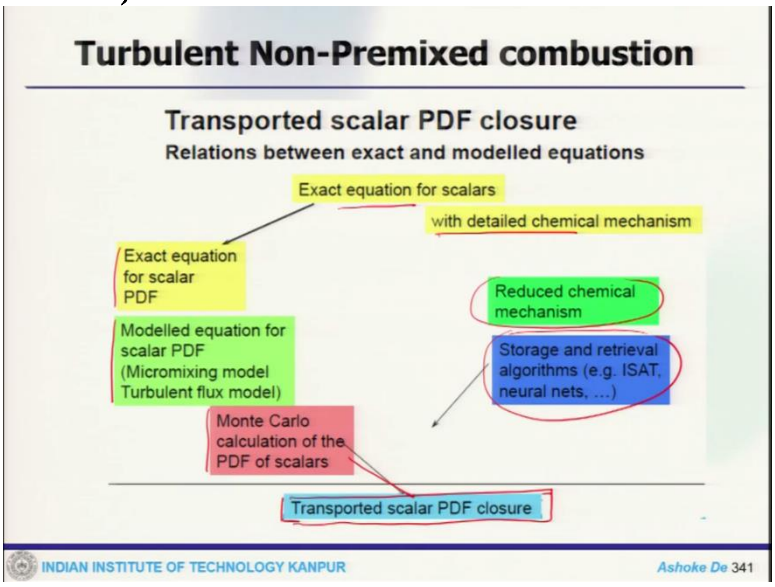

So, you see how we get the equilibrium things and this is transported scalar PDF approach. We get exact equation for scalars with detailed kinetics mechanism. We will get exact equation for scalar PDF. This is the modelled equation where micromixing term and all these then you have Monte Carlo simulation, which will give you this. And these are the kinetic mechanism where you need this storage of and retrieval of the algorithm. That is why the ISAT comes into the picture and this is expensive and we get this transported PDF approach. And the other one can have flamelet / transported z-PDF closure.

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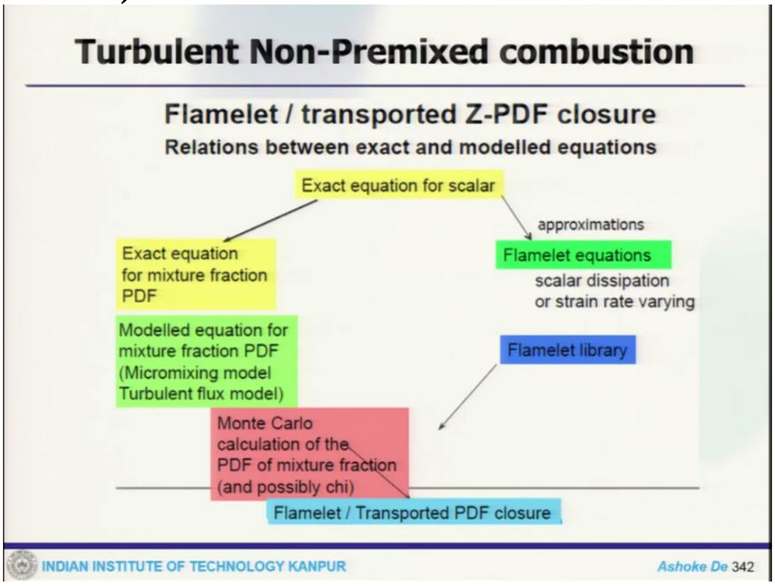

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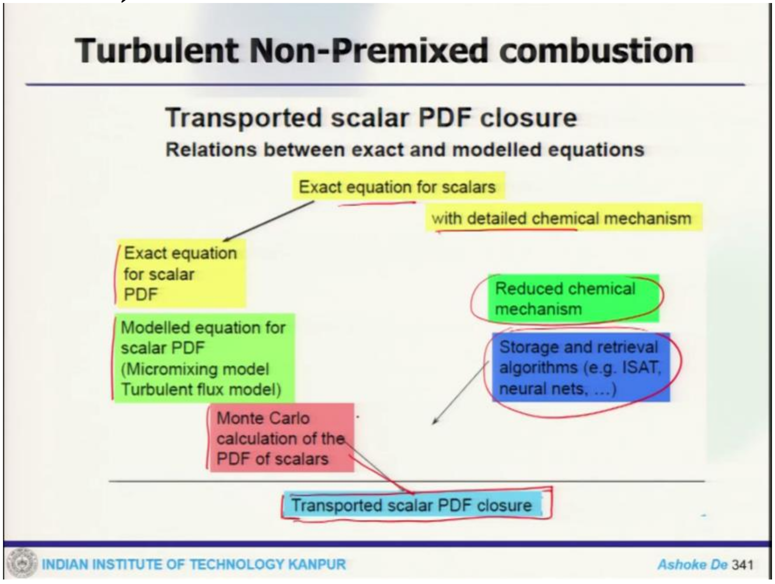

Which means that instead of solving this scalar transported mass transfer equation using the Monte Carlo technique we can close that using the flamelet and how that is done.

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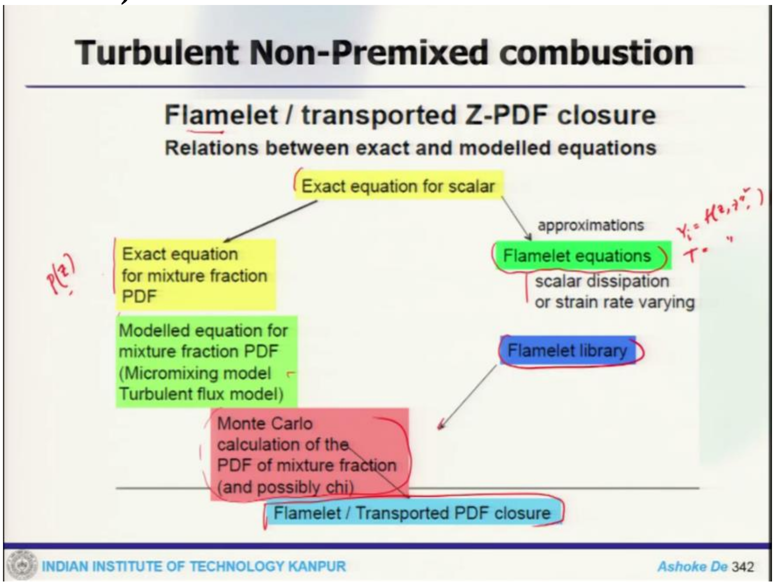

We have exact equations for scalar, now the exact equation for mixture fraction PDF. So, here the PDF is for the mixture fraction. So, that means there is a huge dimensional reduction. On the other hand, we solved the flamelet equation that means, here we get mass fraction is a function of Z, Z variance and like that temperature is also a function of that which is for bearing scalar dissipation rate we get it and we compute the library. Here the PDF function is for Z.

So this is the transport equation or the exact equation for the mixture fraction PDF. So that means instead of and then the model equations where you use the micromixing model, turbulent scalar flux and solve this using Monte Carlo algorithm and using this flamelet library, you get the flamelet transported PDF closure. So, this is what it is doing, it is taking the advantage of the flamelet model and also taking the advantage of the transported PDF model.

So, what it does, instead of assuming the reshape of probability density function of the flamelet, we are here solving the probability density function for the mixture fraction itself. So, this is slightly variant or slightly different from the typical transported PDF approach.

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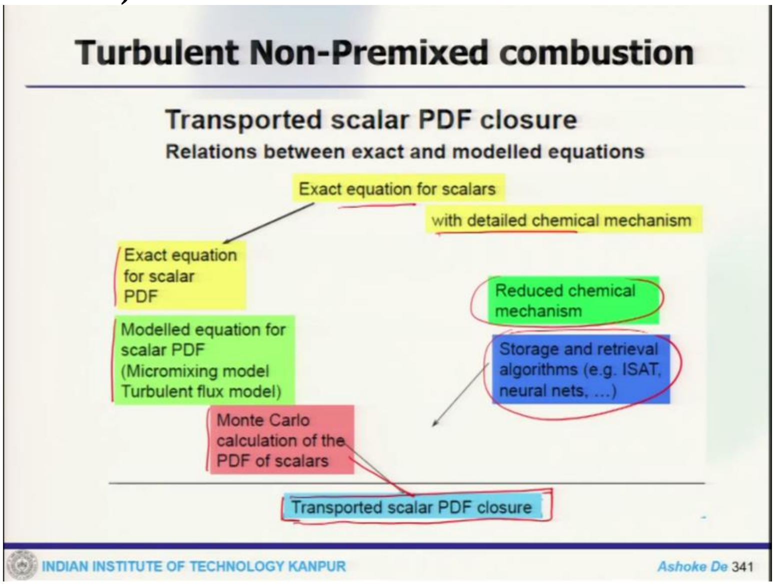

Where you solve for individual scalar equations like mass fraction and temperature in the Monte Carlo algorithm.

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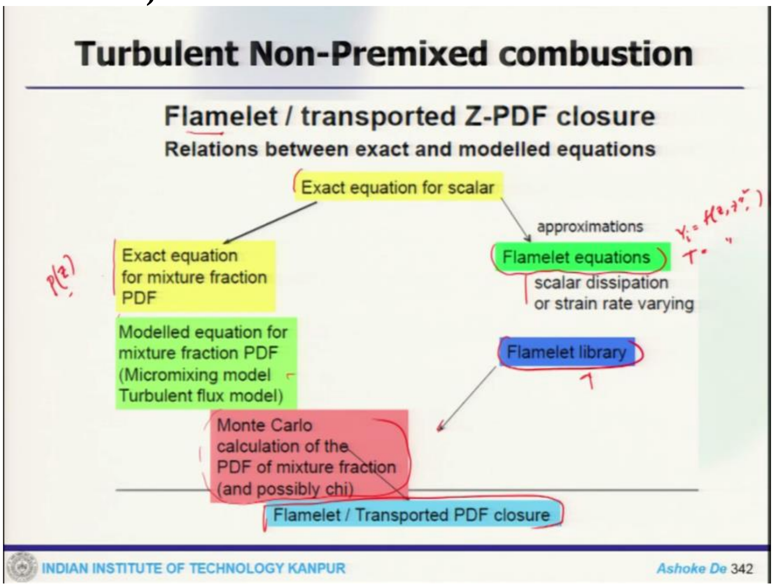

In this particularly this flamelet transport approach here, instead of solving the mixture fraction in Eulerian framework, now probability density function of mixture fraction that we solve in a monte Carlo algorithm and using the information of the library, we close it. So, that is somewhere taking the advantage of this and this tells you how there are different approaches which are available and we have discussed also like equilibrium.

If we just quickly sum up. You have equilibrium based presumed Z PDF closure, then you have flamelet based PDF approach, a flamelet generated manifold kind of PDF approach, then transported scalar PDF closure and the transported z-PDF closure.

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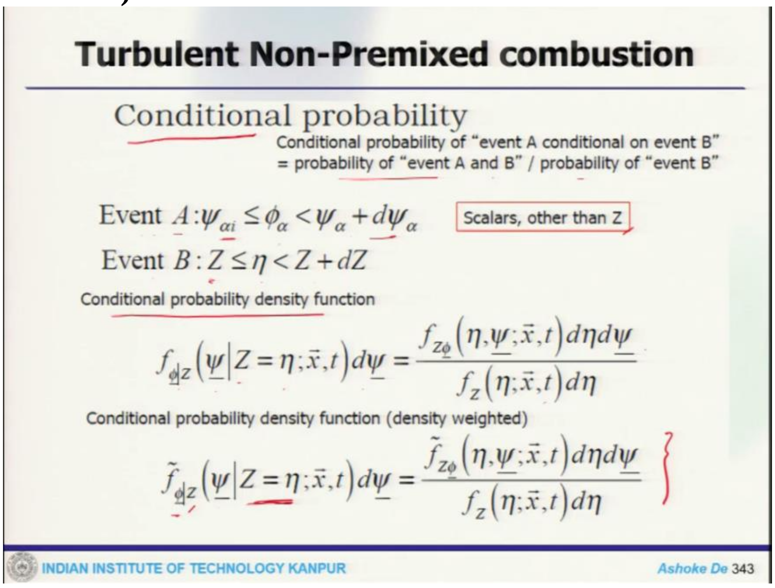

Now we look at the definition of conditional probability. So the conditional probability of event A, conditional on event B would be equals to probability of event A and B divided by the probability of event B. So, let us say scalars which are other than Z event A, which is φ_α which belongs between $\psi_{\alpha i}$ and $\psi_\alpha + d\psi_\alpha$ and for event B, η belongs between Z and Z+dZ. So, this is how finding the probability of η now, the conditional probability density function. How we define that $f_{\phi|Z}$ which is:

$$f_{\phi|Z}\left(\underline{\psi}|Z=\eta;\vec{x},t\right)d\underline{\psi} = \frac{f_{Z\underline{\phi}}\left(\eta,\underline{\psi};\vec{x},t\right)d\eta d\underline{\psi}}{f_Z(\eta;\vec{x},t)d\eta}$$

Now the conditional probability density function density weighted if you write that means:

$$f_{\phi|Z}\left(\underline{\psi}|Z=\eta;\vec{x},t\right)d\underline{\psi} = \frac{\tilde{f}_{Z\underline{\phi}}\left(\eta,\underline{\psi};\vec{x},t\right)d\eta d\underline{\psi}}{f_Z(\eta;\vec{x},t)d\eta}$$

We get the probability of this function. So, this is where you get the conditional probability that means you try to find out the probability density function.

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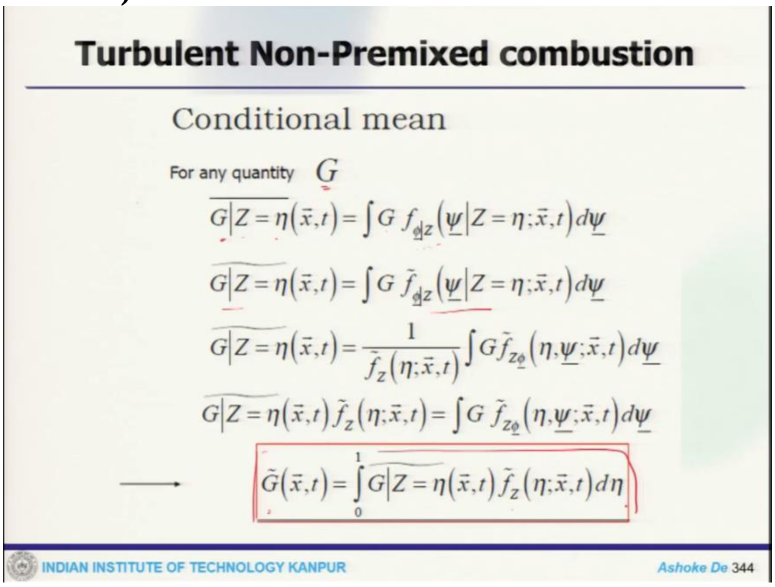

When z equals to eta and this is how you define the density weighted conditional probability. And conditional means similarly for any quantity let us say G. G when it is conditioned at η it would be $\int G f_{\phi|Z}\left(\underline{\psi}|Z=\eta;\vec{x},t\right)d\underline{\psi}$. This is probably, averaged. So, one can find out the mean G go to one G condition that η and $f_Z(\eta;\vec{x},t)d\eta$. So this will give you the mean variable for any quantity and like that.

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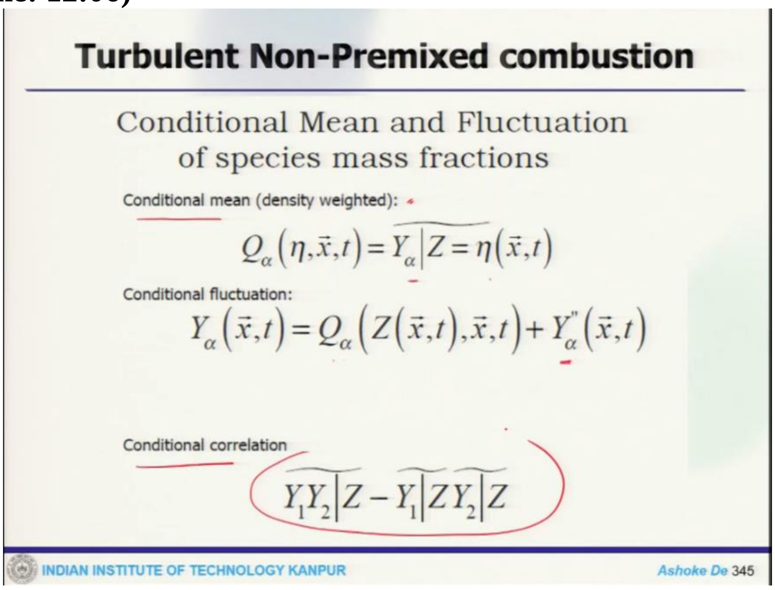

Now, if you look at the conditional mean and fluctuation of species mass fractions. So let us say which to find out the conditional mean are the density weighted mean of Q_α. So, this should be $Y_\alpha|\widetilde{Z=}\,\eta(\vec{x},t)$ Y and conditional fluctuation would be Y_α for $Q_\alpha + Y_\alpha''$. So, the conditional correlation that will remain is:

$$Y_1Y_2|Z - Y_1|ZY_2|Z$$

So, this is the correlation that one has to find out.

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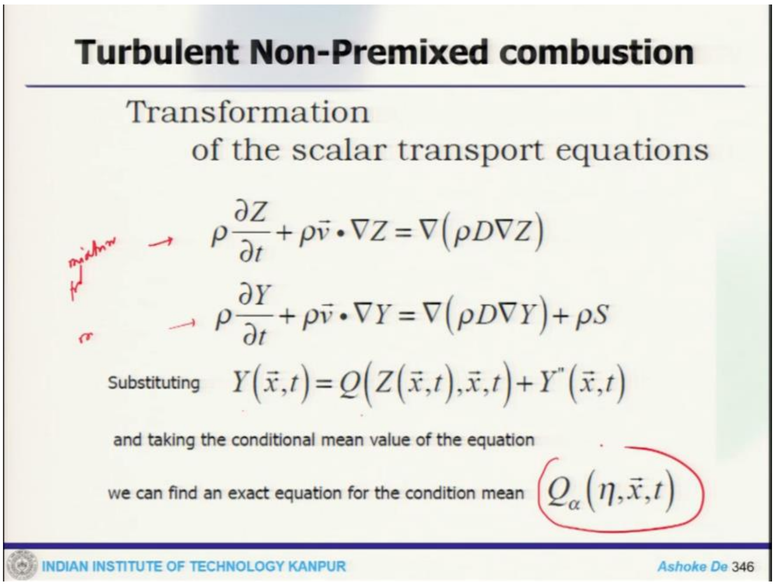

Now we will see the transformation of the scalar transport equations. So, this is on mixture fraction, this is mass fraction. Substituting Y is Q + Y” and taking the conditional mean, we find out the exact equation for conditional mean Q_α.

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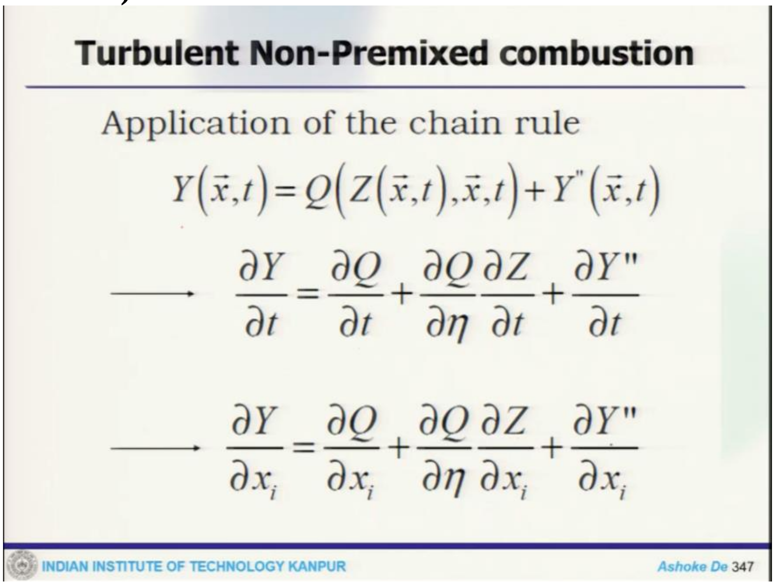

So, application of the General Y is:

$$\frac{\partial Y}{\partial t}=\frac{\partial Q}{\partial t}+\frac{\partial Q}{\partial \eta}\frac{\partial Z}{\partial t}+\frac{\partial Y''}{\partial t}$$

Because Q is now:

$$\frac{\partial Y}{\partial x_i} = \frac{\partial Q}{\partial x_i} + \frac{\partial Q}{\partial \eta}\frac{\partial Z}{\partial x_i} + \frac{\partial Y''}{\partial x_i}$$

So, this is exact equation of the conditional mean.

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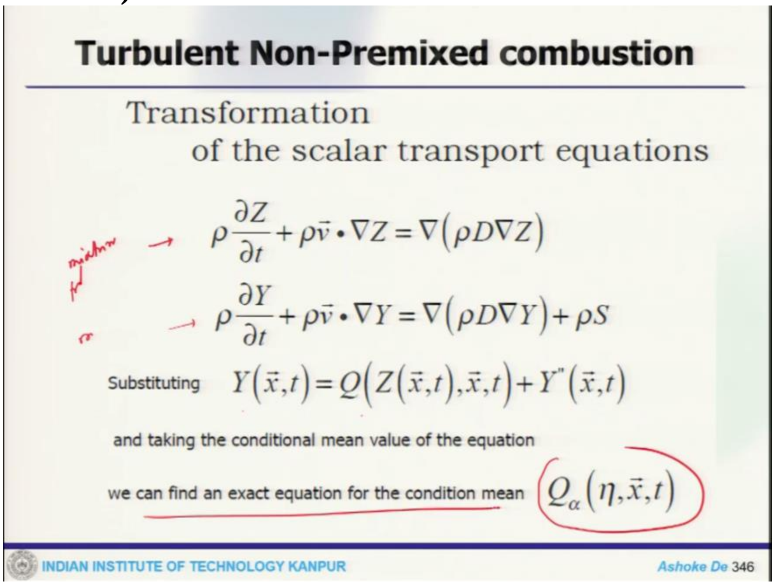

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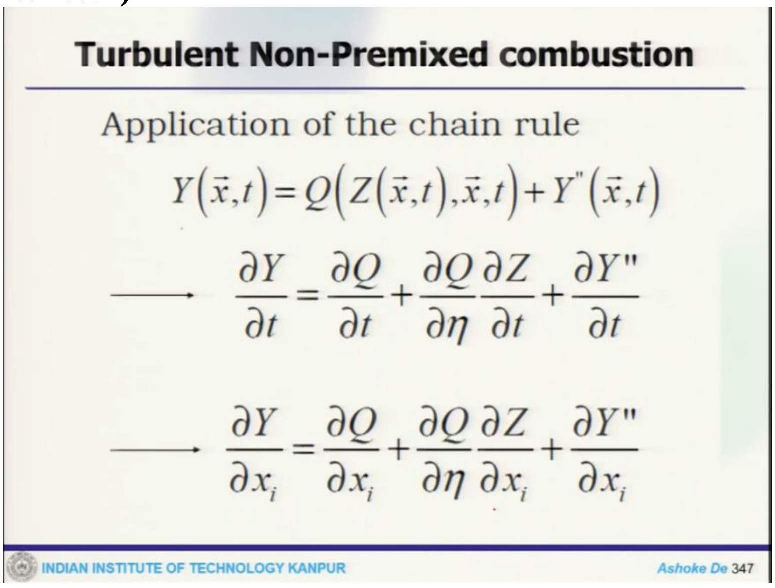

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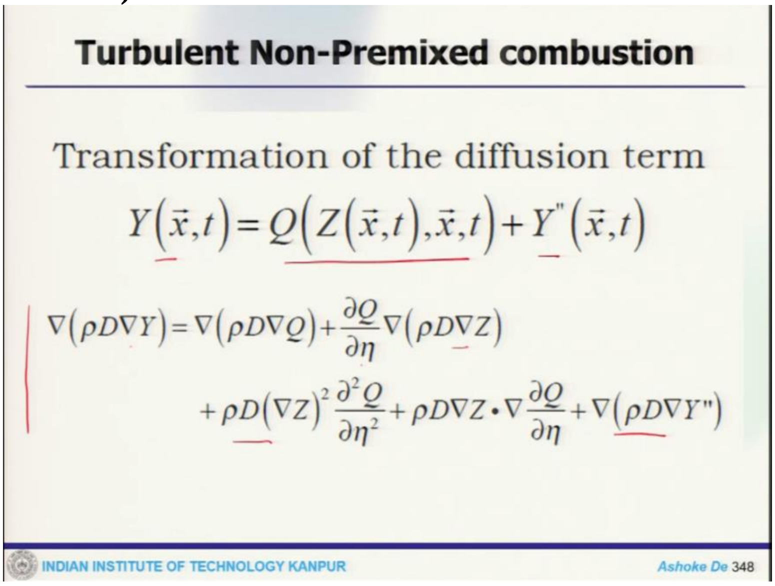

Now that transformation of the diffusion term similarly, we use Y is Q + Y”. So, we write:

$$\nabla(\rho D\nabla Y) = \nabla(\rho D\nabla Q) + \frac{\partial Q}{\partial \eta}\nabla(\rho D\nabla Z)$$

So again we are using the simple chain rule for the derivative and what we get $\rho D(\nabla Z)^2$ which is again the second derivative of $\frac{\partial Q}{\partial \eta}$ and $\rho D\nabla Z.\nabla\frac{\partial Q}{\partial \eta}$. So this is a diffusion term that you get after replacing those conditional information.

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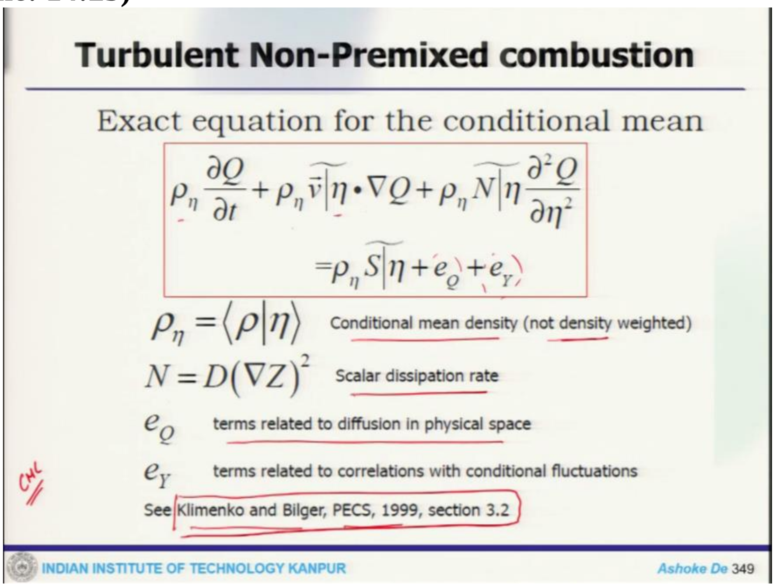

Now you go to exact equation of the conditional mean. So you putting those back:

$$\rho_\eta\frac{\partial Q}{\partial t} + \rho_\eta\widetilde{\vec{v}|\eta}.\nabla Q + \rho_\eta\widetilde{N|\eta}\frac{\partial^2 Q}{\partial \eta^2}$$

So this the term what you get $\langle\rho|\eta\rangle$ is the conditional mean density, not density weighted so mind it. This is ρ when Z equals to η that is a condition N is $D(\nabla Z)^2$. This is a scalar dissipation rate e_Q, which is a terms related to diffusion in physical space.

That is this term e_Y which is the term of conditional fluctuation. Now one can look at the equations of this paper in PECS progress in Energy and combustion science, about there is this particular literature which is quite important, which will give you an complete idea about these CMC model description and all these. So, which will let you to get into these details these are.

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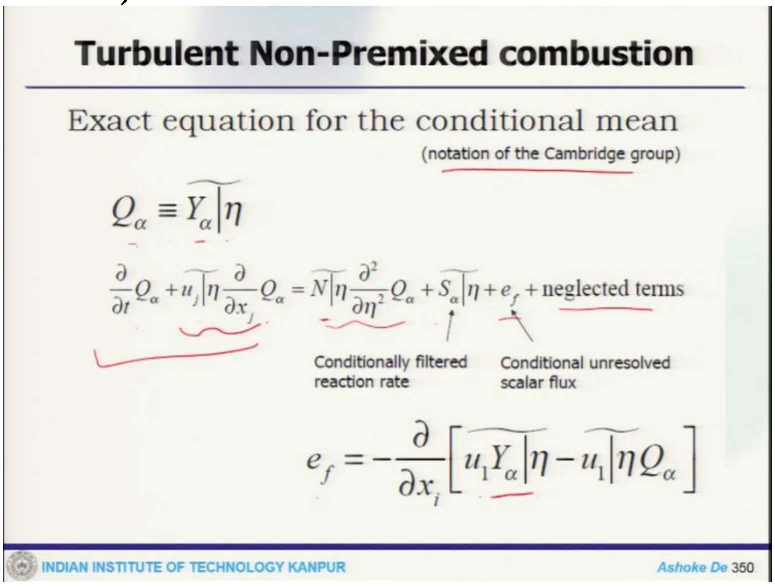

Now, if we come down to the exact equation for the conditional mean you have the notation of the Cambridge group is in the similar notation we write:

$$Q_\alpha = \widetilde{Y_\alpha|\eta}$$

That means this is the conditional mean. So, our equation will become like this. So, this looks like and similar to our convection term and the total left hand side looks like in derivative. Total derivative but obviously condition and this looks like a conditional density a conditional diffusion term, this is a conditionally filtered reaction rate term, and conditional unresolved scalar flux term which are neglected terms and what e_f contains:

$$e_f = -\frac{\partial}{\partial x_i}\left[u_1\widetilde{Y_\alpha|}\eta - u_1\widetilde{|\eta Q_\alpha}\right]$$

So, this is the term which has to be closed.

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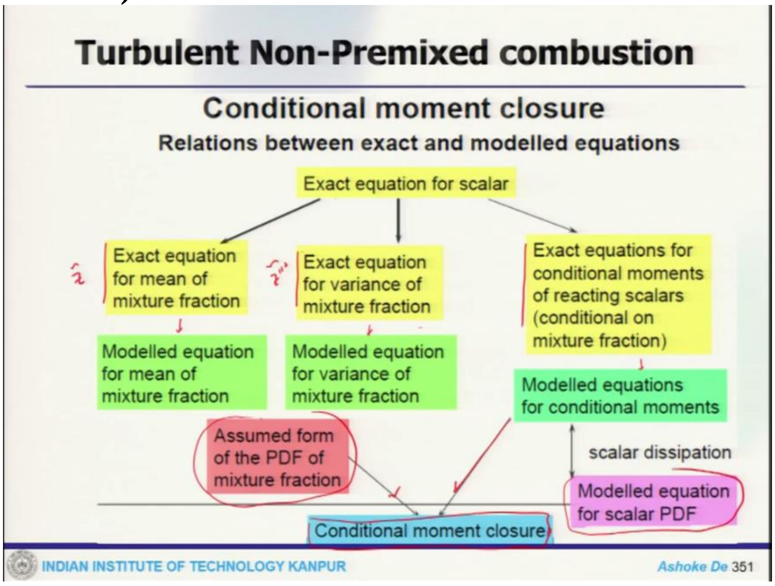

If we see this conditional moment closure things and the connectivity between these different things, we can quickly see there is an exact equation for the scalar. Now, from there, you get exact equation for variance of the mixture fraction and then you have exact equation for mean or mixture fraction. So, this is what you get. This is mean, this is variance Z an exact equation for conditional moments of reacting scalars.

So, these are conditional mixture fraction. From there, you get the mean quantity model equation for mean of mixture fraction for the variance and the conditional moments. Now, you have an assumed PDF for the mixture fraction. Here you can have modelled equation for scalar PDF and which goes to the modelled equation. And using these 2 information, you finally get the CMC closure.

So, this is slightly different from the other things that we have already discussed, because this uses a different sort of information to closure terms like that. So that is why one has to be bit careful because this is also be involved in computational. This is also slight delay I mean this is not expensive like transported PDF approach, but this is also quite expensive computationally and but provide you very good prediction.

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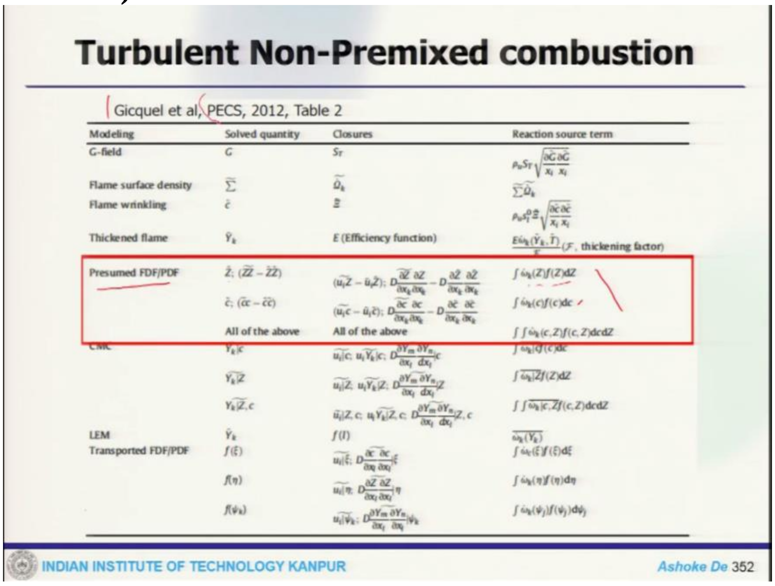

Now, from this literature that table and this will give you an idea what we do, when you look at the presumed probability density function or PDF function, you solve for ZZ variance c variance and all this then you have closures for all these like gradient diffusion assumption and then finally source terms for using the PDF function. Now, the details you can find out this literature.

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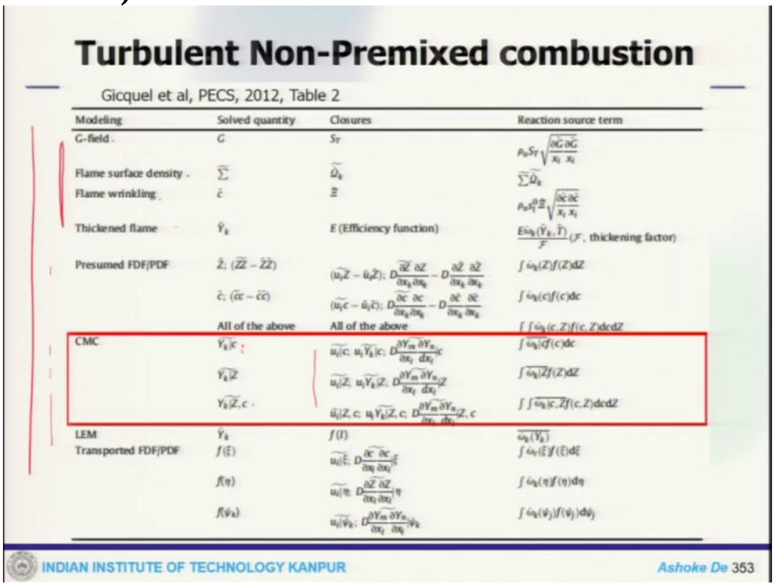

Now, when you come to this table actually quite good or informative in the sense this is actually taking into account the kind of discussion that we have hide that different kind of like this is G equation for previous case thin surface density for premixed case wrinkling factor taken flame. So these are the models which are actually for pre-mixed case and they compare how they compare to each other.

Then we come to the non-premixed case. We can compare how so this is when the CMC, you have conditional mean a mass fraction, then the conditional at Z and c and then you actually close these terms or condition terms, and then finally, close the source term. So, this is how in CMC, you take into account.

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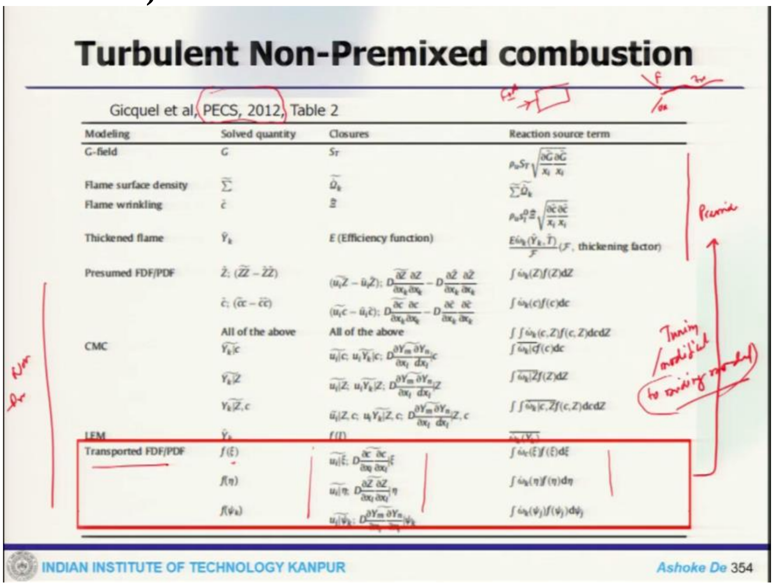

Now, when you go to transported PDF You have solved for $f(\xi)$, $f(\eta)$ and $f(\psi)$, and then you close these terms using your information and finally, you get those reaction and source them closure. So, one I would suggest that you should go through this particular literature. This is in progress in energy and combustion science in 2012. This will give you a good overview of all these models that we have been talking and how there are different terms which are unclosed and how they are closed.

So, sort of getting you in nice overview of everything. So, that is what is important, because already you can see upper half talks about the pre-mixed case and the lower half talk about the non-premixed case. Specifically, if you look at this, again as I mentioned this is theoretical description or theoretical system, it is suggested or said that it can be applied to any mode combustion. But when it comes to the application of premixed combustion it requires some fine tuning specially in the mixing model term. Rest of the terms appear to be okay but when you apply to this one in the premixed case, so you require tuning or modification to mixing model because the mixing model thing or the concept of the mixing model is actually is missing in premixed case.

Because in diffusion flame, one of the ideas is that your fuel and oxidizer are injected separately. So, they come through the molecular mixing, and then allowing the Z stoichiometric reaction takes place, but in premixed case everything is injected by pre mixing, so the fuel and air they are pre mixed. So that is why the concept of this mixing model is little bit not that real to be applied in the case of premixed combustion. And that is why there are a few literature where there were people have tried to modify in terms of premixed flame, how one can do that. So that is another important aspect of it.

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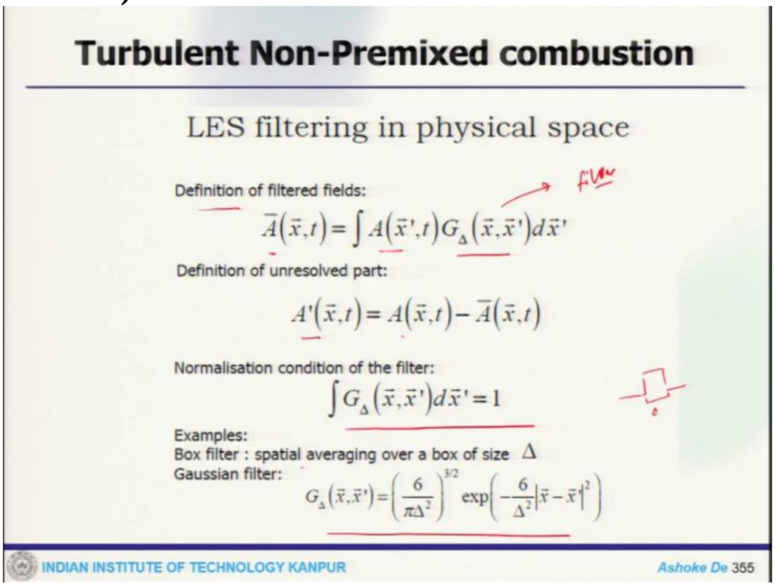

Now, just to final to conclude before these things we will look at the now because all of our discussion pretty much kind of restricted looking at the RANS framework, but in the earliest case, this should be filtered function where the filtered field would be integration of A and this is the filter which you use. So, the definition of unresolved part which is A’ – A mean and if you will normalize the filter this would satisfy this property and there are different kind of filter and their box filter.

So, this a box filter. It does spatial averaging over a box of size Δ. So, that means, these kind of things then there could be Gaussian filter which looks like in distribution of a Gaussian kind of distribution over a filter size are Δ.

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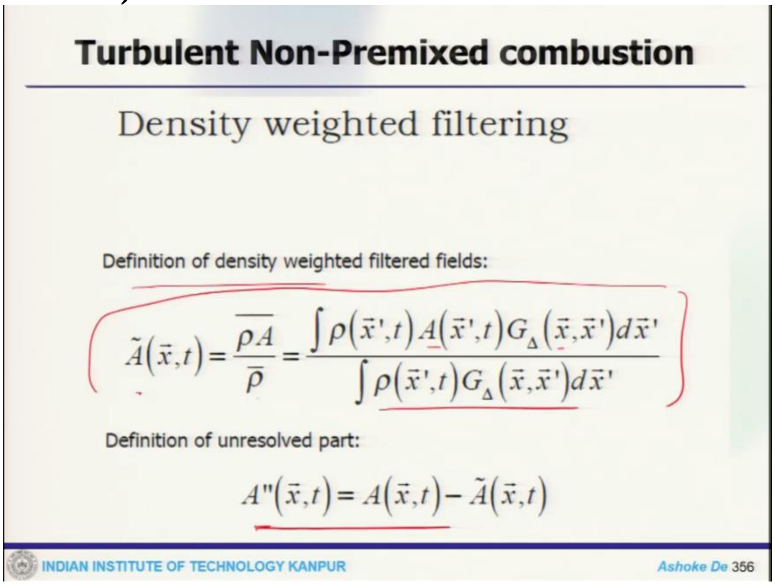

Then once you define some filter, you can actually defined some density weighted filtering that density weighted filtering look like rho A bar by rho bar rho it is integrated over filter. And this is what one has to use, again because it is a reacting system. So, instead of these that density weighted filtering is what is more appropriate. Then you resolve this is similar to that RANS things where we have density weighted filtering, here we are using density weighted filtering. So that you get the effect of density due to temperature variation and so.

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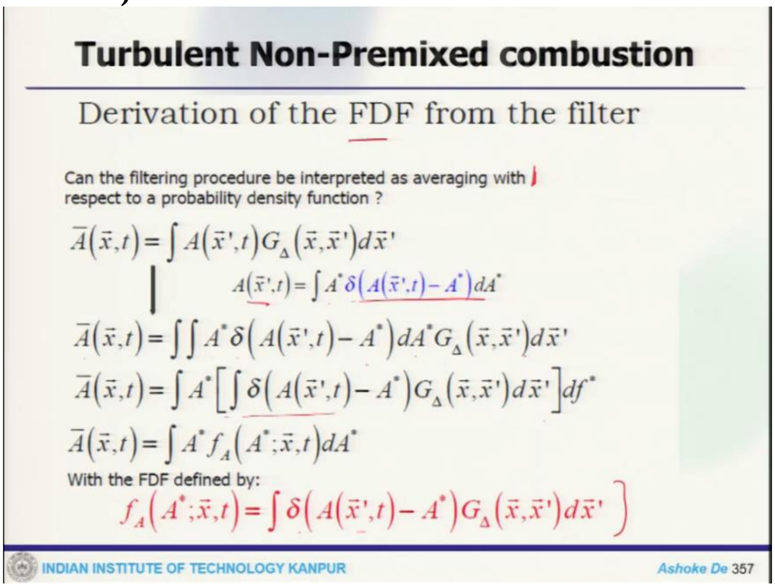

Now, if I derive the filter density function, this is filter density function. From the filter, can the filtering process be interpreted as everything with the respect to probability density function? So that is a question and we can see whether it is true or not. So this is our mean and the mean is obtain like A and G Δ. Now, this A one can right is that the A*δ of the A*.

Once we put that back that mean it will become double integration of A*δ function A* and the filter function which will become this quantity if it take into the bracket and the mean will become with the filter density function defined f_A which is then δ function and the δ function. So, that is what one can actually replace this filter quantity by n probability density function.

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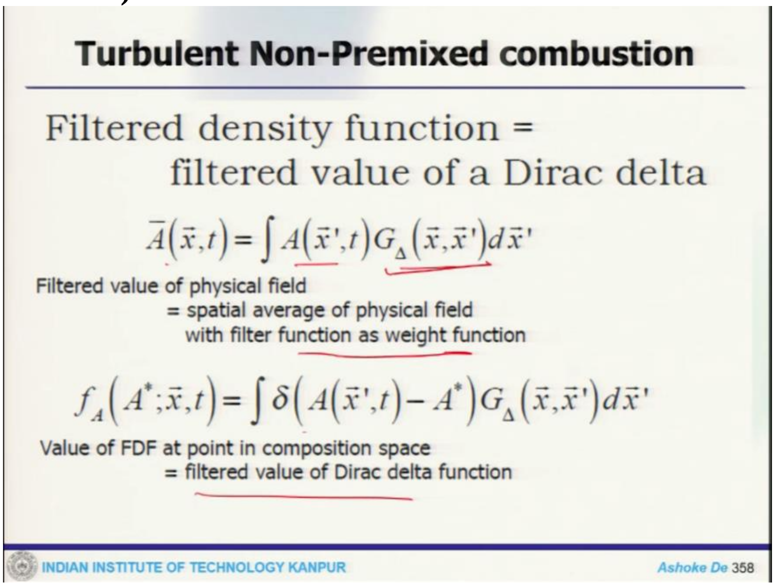

Now, the filter density function is essentially filtered value of a Dirac delta function. So if you have this A, which is A and G_Δ, so filtered value of the physical field that spatial average of the physical field with filter function as a weight function. So this a weight function. It is essentially though we are talking about so many mathematical description, integration and all these things, but it boils down to and this is an important statement is boiled down to a numerical integration of some weight function.

So the probability function would be defined as the δ function. So the value of FDF at point in composition space would be the filtered value of the Dirac delta function. So all these different kind of delta functions, they are nothing but just sort of you can think about the different what a filter size of δ that we the weight function is used to get the filtered quantity.

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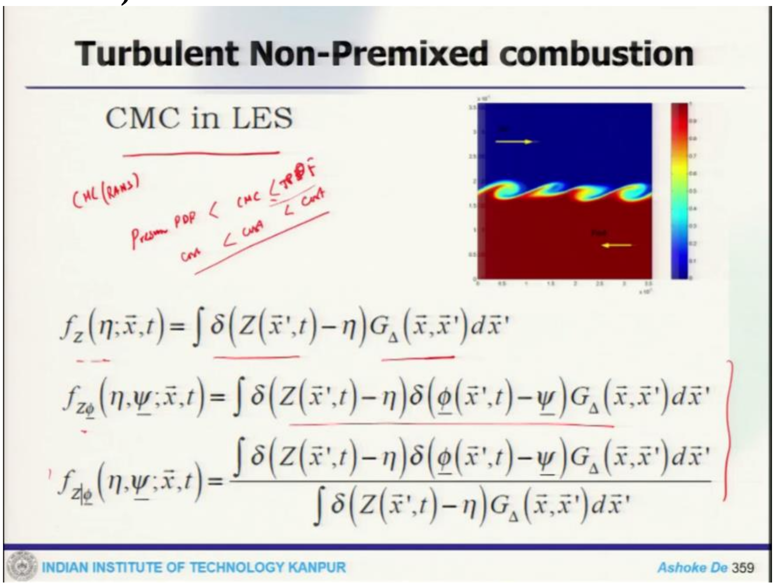

And now similarly, like your RANS framework, this is an example often these things, one can use also an LES framework and CMC. So, CMC in RANS is itself quite computationally expensive, but when you go to an LES, it will become more computationally expensive. So that the price you pay, but this can provide you good prediction compared to so if you have presume PDF.

So, the CMC would be better or rather sometimes equivalent to transported PDF. But if you look at the computational cost this is the low cost. Here, the cost would be high. Here, the cost is much higher. So, the cost wise also, but this can provide you very computable regular like a transported PDF of approach, but it is that is why it is equal, but this is very specific to non - premixed case.

So now once you go to LES come situation, this will actually be more distinct. So, the f_z for to have this you can use the δ function with this filter function and the probability distribution function, which could be written like this. And finally, the condition one can write like that. So, that is how you can define this CMC equations in RANS and LES framework.

So that is pretty much concludes the discussion on our gaseous part of the combustion modeling where we have looked at premixed and non-premixed case. Now we will stop here today, and we will continue the discussion for multiphase flow in the next lecture. Thank you.