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

Lecture-52
Turbulence-Chemistry Interaction (Contd...)

Welcome back. So, we are in the middle of the discussion of this G equation or level set based approach, where we have already looked at the D equation for the corrugated flamelet regime. And also we have seen how G equation actually differs on you go to thin reaction zone regime. Now, we would like to see how you can combine these 2 and come up with 1 equation, which will be applicable to both the regime.

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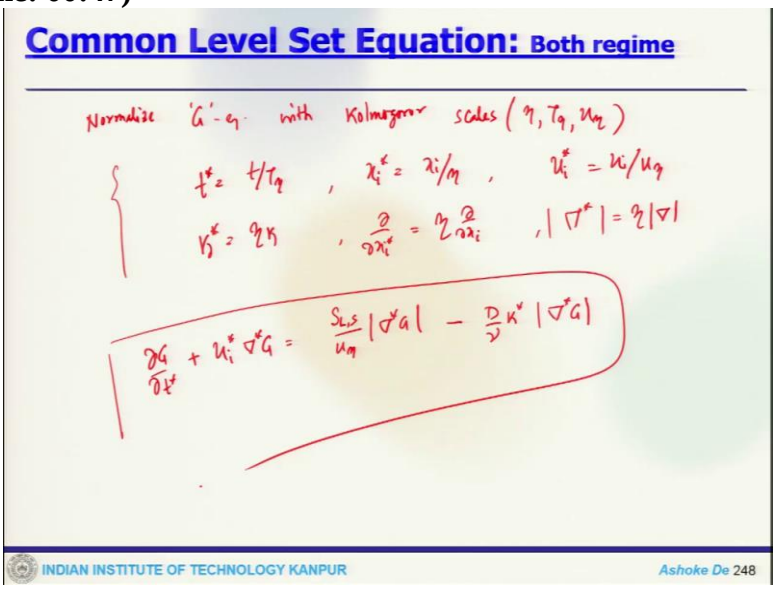

So, we will normalize the G equation with Kolmogorov scale like η, timescale, u_η. Our t* would be t/T_η, x_i^* would be x_i/η, u_i^* would be u_i/u_η. And κ^* would be $\eta\kappa$, $\frac{\partial}{\partial x_i^*}$ is $\eta\frac{\partial}{\partial x_i}$ and $|\nabla^*|$ is $\eta\nabla$. So, now if I use this normalization parameters, which you can write the G equation like:

$$\frac{\partial G}{\partial t^*} + u_i^*\nabla^* G = \frac{S_{L,S}}{u_\eta}|\nabla^* G| - \frac{D}{\nu}\kappa^*|\nabla^* G|$$

So, this is what we can write.

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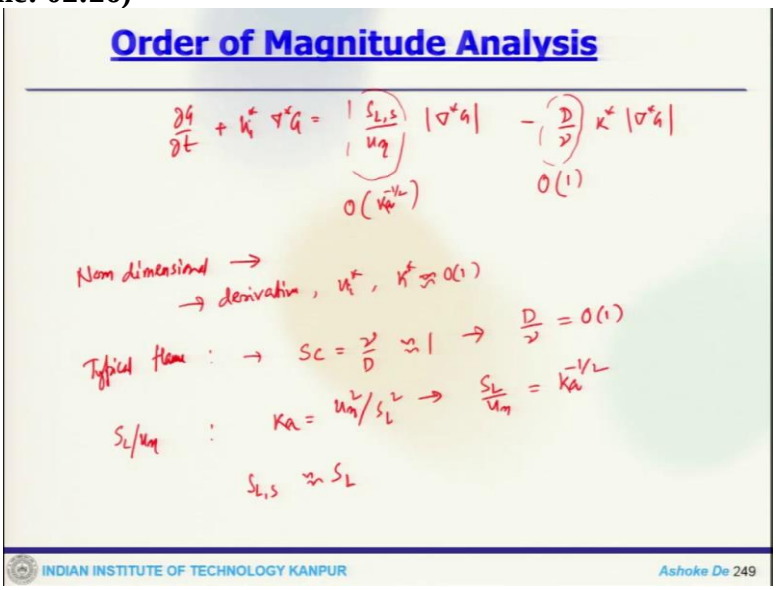

We look at now, some order of magnitude of this term. So, this is the equation we are now dealing with this is:

$$\frac{\partial G}{\partial t^*} + u_i^* \nabla^* G = \frac{S_{L,S}}{u_\eta} |\nabla^* G| - \frac{D}{\nu} \kappa^* |\nabla^* G|$$

Now we have this term and look at this term. So, this is order of Karlovitz number to the power –1/2. And this guy is order of 1. So, if we non-dimensional thing the derivatives and u_i^*, κ^* which will be order of 1. So, we can see this non-dimensional form of these things.

Now, if you look at typical flame what will happen? That $Sc = {}^{\nu}/_{D}$, which is 1 that means ${}^{D}/_{\nu}$ would be order of 1. And S_L/u_η and Karlovitz number is u_η^2/S_L^2. So, S_L/u_η is Karlovitz to the power –1/2 and $S_{L,S}$ will be order of S_L.

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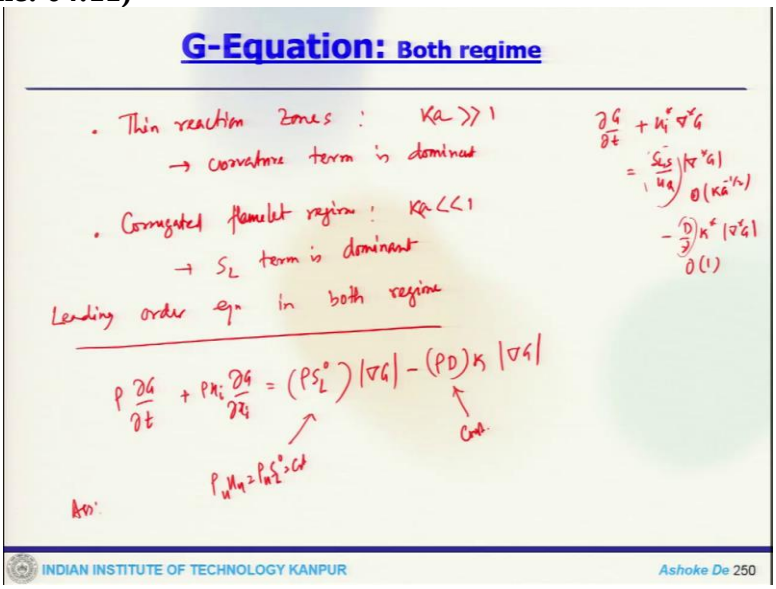

Now, one can see when a thin reaction zones where your Karlovitz number is greater than 1 so your curvature term is dominant. Why? Because if we look at that equation:

$$\frac{\partial G}{\partial t^*} + u_i^* \nabla^* G = \frac{S_{L,S}}{u_\eta} |\nabla^* G| - \frac{D}{\nu} \kappa^* |\nabla^* G|$$

So this is order of $\left(Ka^{-1/2}\right)$. This is order of 1. So, when you go to thin reaction zone if kappa is too high, so it is the curvature which will dominant. Now at the same time if you go to corrugated flamelet regime where Karlovitz number is very small. This term is going to be dominant. So S_L term is dominant. So, if you take the leading order equation in both regime. So you can write:

$$\rho \frac{\partial G}{\partial t} + \rho u_i \frac{\partial G}{\partial x_i} = \rho S_L^0 |\nabla G| - (\rho D) \kappa |\nabla G|$$

So, this term with the assumption that $\rho_u u_u = \rho_u S_L^0$ which is constant and this is also constant. So, now, we can use our knowledge of statistical description and we can actually define this.

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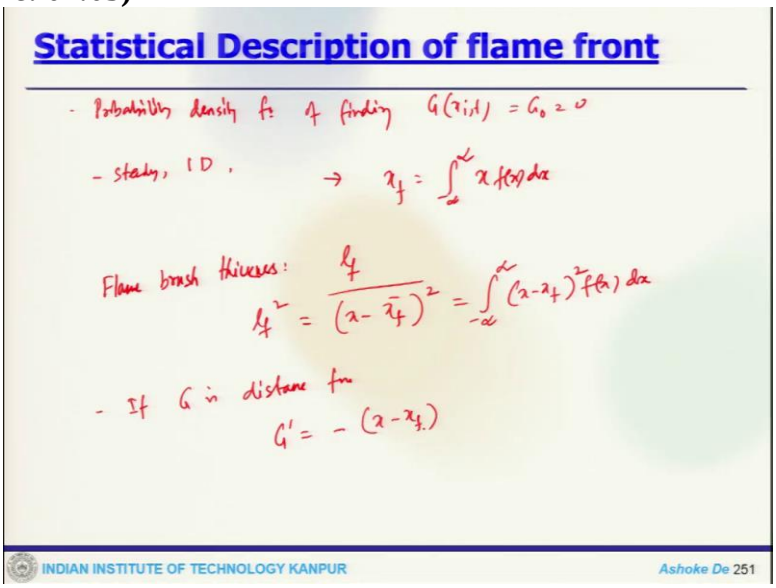

Now we can see the probability density function of finding G, which is G not equals to 0. So, if you consider and study one dimensional premixed flame at position x_f where x_f is:

$$x_f = \int_{-\infty}^{\infty} x f(x) dx$$

Now you can define the flame brush thickness, which is l_f. So,

$$l_f^2 = \frac{l_f}{\left(x - \bar{x}_f\right)^2} = \int_{-\infty}^{\infty} \left(x - \bar{x}_f\right)^2 f(x) dx$$

If G is distance function, what we get G prime is –(x – x_f).

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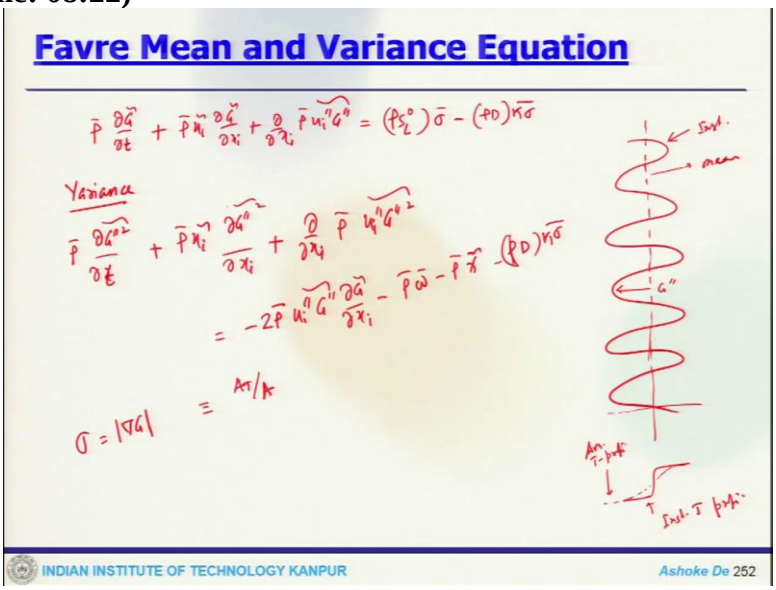

Now, this is the flame front, this is the instantaneous flame front and then this is the mean. This is instantaneous, this is mean. So, one can think about G'' and if you see this, this is what is going to happen. So, this is our average T profile. This is instantaneous T profile. Okay. So you can write for the Favre mean equation, which is:

$$\tilde{\rho}\frac{\partial \tilde{G}}{\partial t} + \tilde{\rho}\tilde{u}_i\frac{\partial \tilde{G}}{\partial x_i} + \frac{\partial}{\partial x_i}\bar{\rho}\widetilde{u_i''G''} = (\rho S_L^0)\bar{\sigma} - (\rho D)\overline{\kappa\sigma}$$

And along with that we get or write another equation, which is in terms of variance. So the variance equation is:

$$\tilde{\rho}\frac{\partial \widetilde{G''^2}}{\partial t} + \tilde{\rho}\tilde{u}_i\frac{\partial \widetilde{G''^2}}{\partial x_i} + \frac{\partial}{\partial x_i}\bar{\rho}\widetilde{u_i''G''^2} = -2\bar{\rho}\widetilde{u_i''G''}\frac{\partial \tilde{G}}{\partial x_i} - \bar{\rho}\bar{\omega} - \bar{\rho}\bar{\kappa} - (\rho D)\overline{\kappa\sigma}$$

Here σ equals to $|\nabla G|$. So this can be interpreted as an area ratio of the flame front A_T/A and variance actually described the average sides of the flame. Now in the variance equation there are terms like seem terms.

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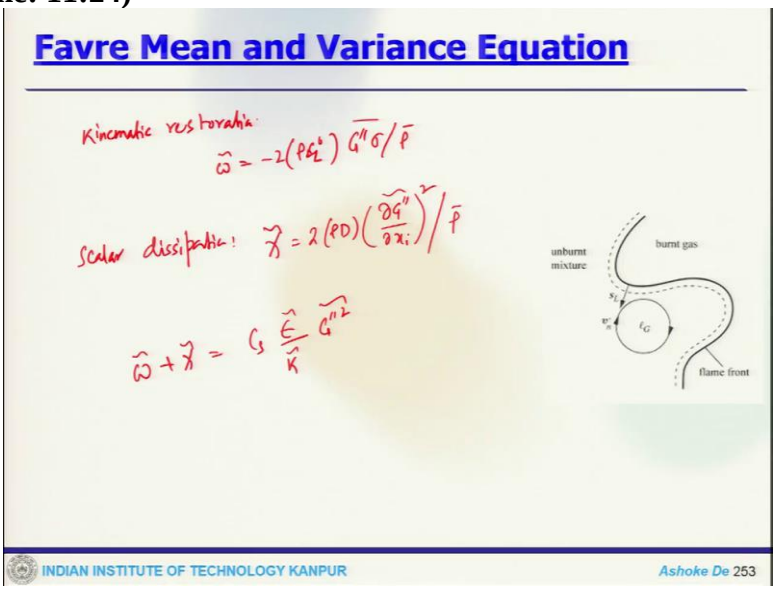

So, the terms which is the kinematic restoration it is this which is $-2(\rho S_L^*)\overline{G''}\sigma/\bar{\rho}$. Scalar dissipation term which is $2(\rho D)\left(\frac{\partial \widetilde{G''}}{\partial x_i}\right)^2/\bar{\rho}$. And these are 2 richer modelled as ω+X. This is $C_s\frac{\tilde{\epsilon}}{\tilde{\kappa}}\widetilde{G''^2}$. So, this is how one get some closer approximation for that. Now we invoke the information of the turbulent burning velocity.

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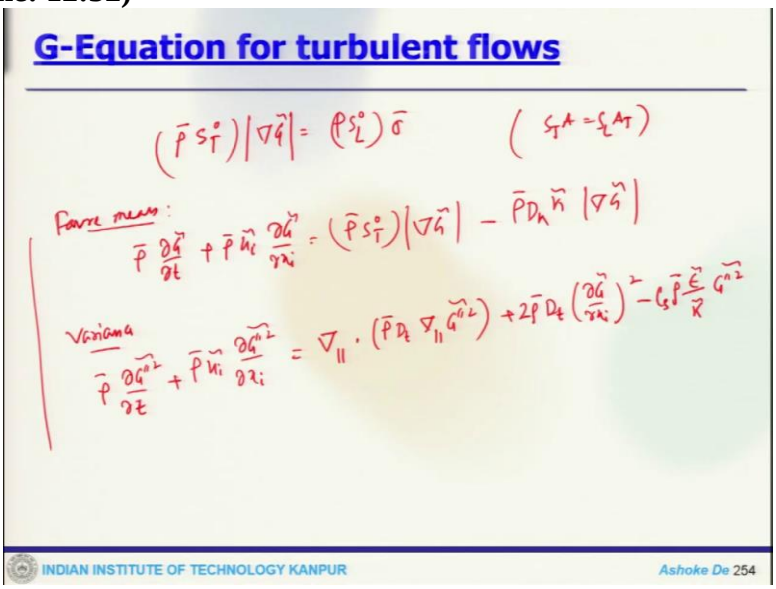

So then we can write:

$$(\bar{\rho}S_T^0)\left|\nabla\tilde{G}\right| = (\rho S_L^0)\bar{\sigma}$$

Here we can say S_TA equals S_LA_T. Now the Favre mean equation will get:

$$\bar{\rho}\frac{\partial \widetilde{G''^2}}{\partial t} + \bar{\rho}\tilde{u}_i\frac{\partial \widetilde{G''^2}}{\partial x_i} = \nabla_{11}.\left(\bar{\rho}D_t\nabla_{11}\widetilde{G''^2}\right) + 2\bar{\rho}D_t\left(\frac{\partial \tilde{G}}{\partial x_i}\right)^2 - C_s\bar{\rho}\frac{\tilde{\epsilon}}{\tilde{\kappa}}$$

So this is what we get 2 equations in that form.

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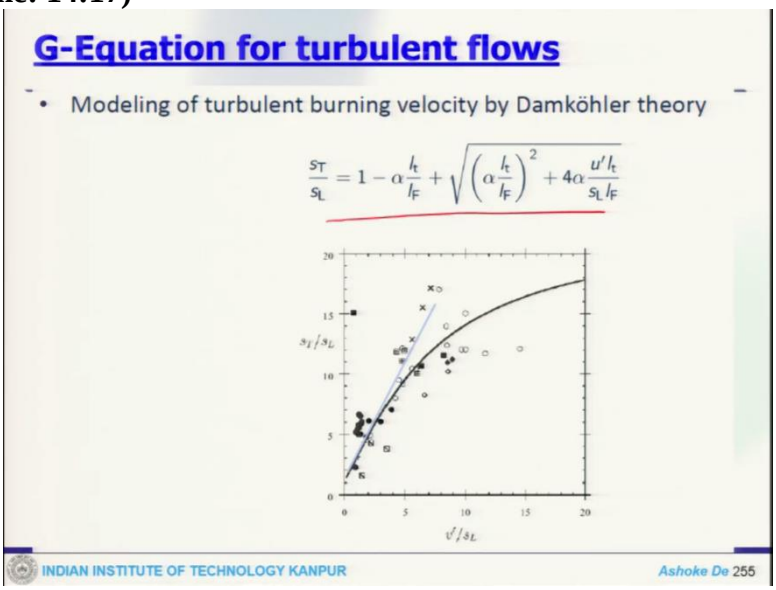

So, now, we have used them turbulent burning velocity expression using the Damkohler theory, and you can see how S_T/S_L actually varies.

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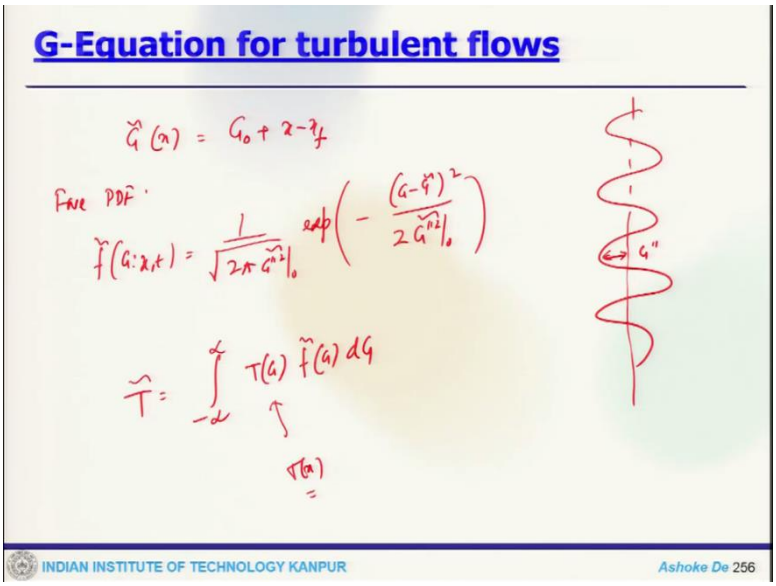

And that is we want to bring in this is the mean. This is the G'. So the Favre mean $\tilde{G}$ is:

$$\tilde{G}(x) = G_0 + x - x_f$$

So the favre PDF would be:

$$\tilde{f}(G:x,t) = \frac{1}{\sqrt{2\pi\left|\widetilde{G''^2}\right|_0}} exp\left(-\frac{\left(G-\tilde{G}\right)^2}{2\left|\widetilde{G''^2}\right|_0}\right)$$

So, now we can find out the mean temperature or any other scalar like this:

$$\tilde{T} = \int_{-\infty}^{\infty} T(G)\tilde{f}(G)dG$$

So, this guy is the T(x) from the laminar premixed flame without strain. So, you can use this and correlate these things.

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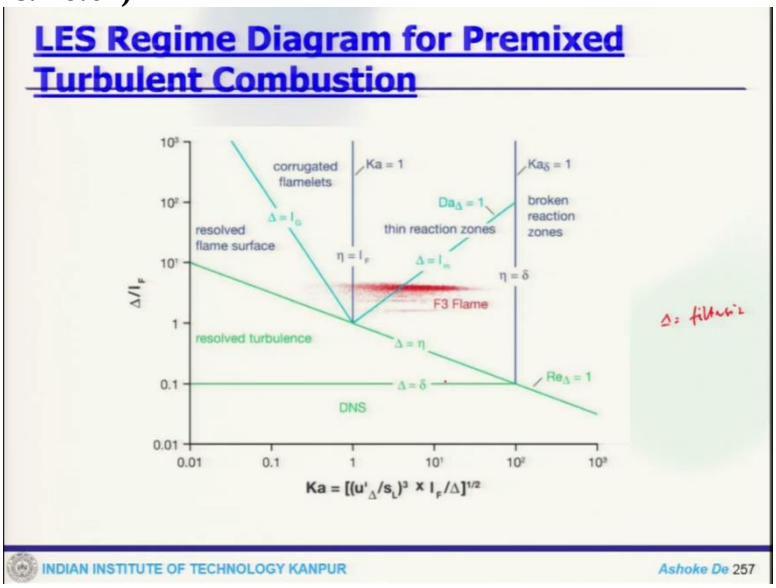

Now, this is how one can use this G equation thin and now when you go to LES for this premixed combustion diagram that gets slightly modified where this Δ is your grid size or filter size and you can use different things.

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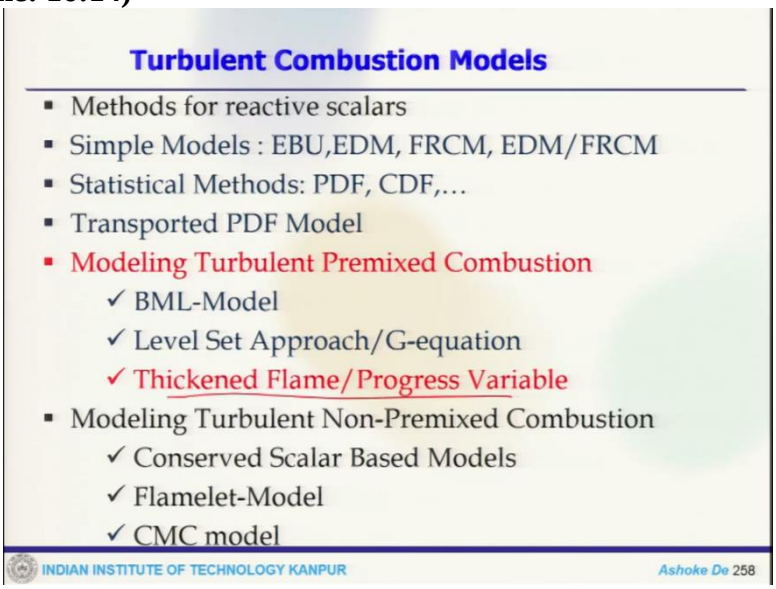

So, that brings to the other part of these things which is thickened flame or progress variable kind of situation. Progress variable we have looked at it. Now look at the thickened flame based approach, which is also very much applicable to.

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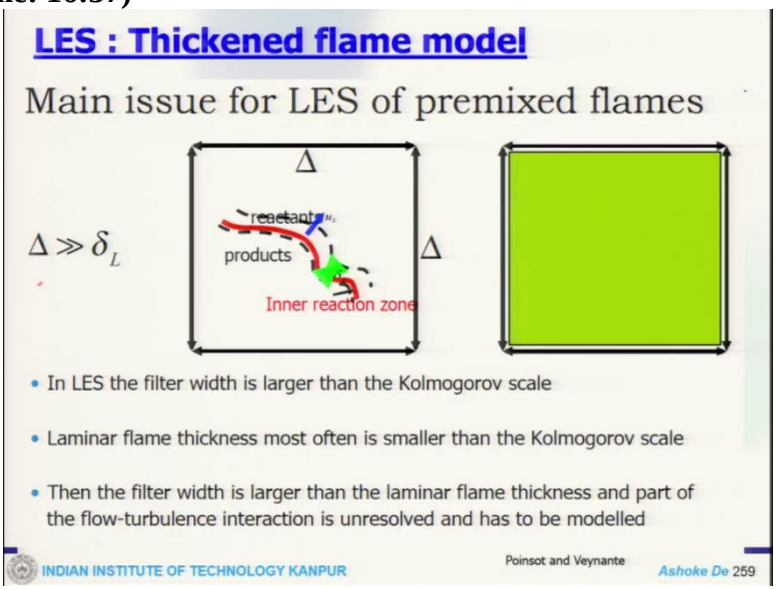

Now, one important point to note here is that, this thickened flame kind of approach is only applicable in the premixed flame front. So, this is not very much applicable in the RANS application is taken from kind of approach. Now, what happens here, as we have said that laminar flame thickness, which is our premixed flame thickness is quite smaller, and sometimes it may be possible that the flame front actually lives within the grid cell which is order of this. So that means one small computational grid is quite larger than this flame thickness. So, then the question is that, how do we capture this flame front?

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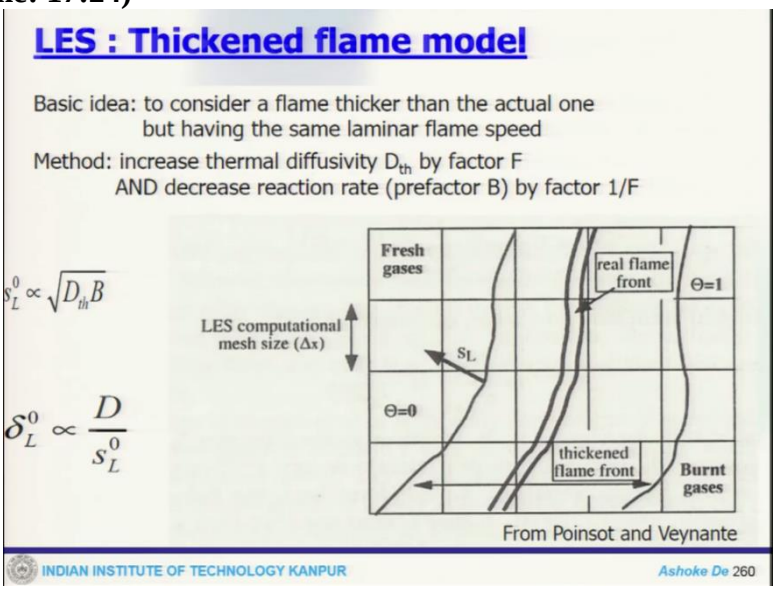

So the idea behind is that you have a very thin flame front, which cannot be resolved on the computational grid. So what is idea is that if we actually artificially that, so it is called also artificially thickened flame model ATF. So the whole idea is that if we actually artificially modify the flame front, that means, for example, this is our grid, and this is our flame thickness. Now, what do you want to do that you modify that thing, and the flame front is thick, so once that happens, then we can resolve that flame front thickness in the grid.

So the whole idea is that if we artificially thicken the flame front, then we will be able to resolve in the computational mesh. Now the point comes how one can artificially thickened the flame front. So, the whole idea behind that thing is that the way this thickening is done that it does not change the basic flame properties like laminar flame speed and flame thickness. So, the flame thickness is typically is a ratio of diffusivity and a ratio of the flame speed of flame speed is that diffusivity in the reaction rate.

So, the way thickening is done. So, if you look at this if you artificially only thicken the flame front by in factor A, then the speed will be reduced by that factor. So, to avoid that thing, the thickening is done in such a way that you increase this diffusivity by a factor F at the same time. So, essentially the suit like an S_L not would you look like F into D_{th} into B by F. That means at the same time you reduce the reaction rate by same factor that the way it is done, it does not change those properties.

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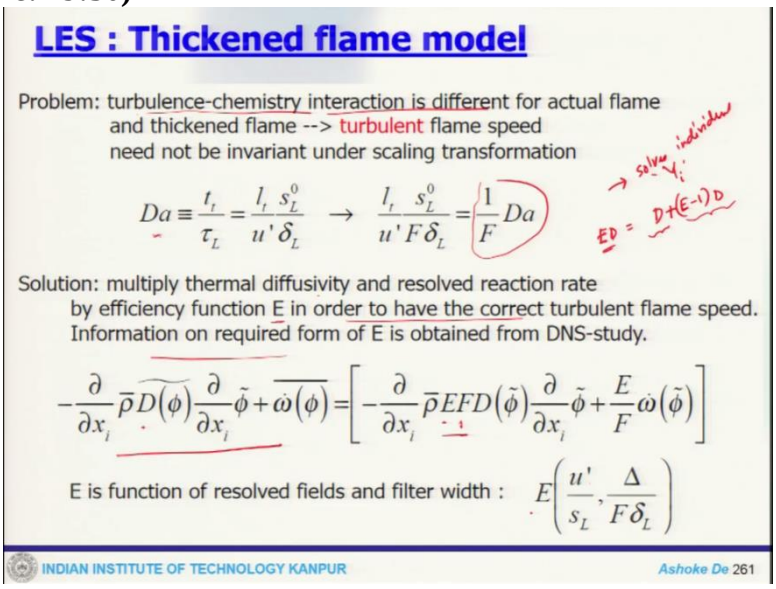

So, by doing that so, which means the unthickened flame front or thickened flame front is not going to behave in the similar fashion that like the actual flame front use to behave. So, now, once the flame front is thicken this is not going to behave like to the actual flame front. So, the turbulent flame speed need to be invariant under the scaling transformation. Now, if we look at the Damkohler number, which is an issue of low and the scale, so, these also gets reduced by n factor.

So, the solution to that because that means, we are by artificially changing the flame front also we are changing the some of these properties, we are changing the Damkohler number of the flame front, so, it may belong to a completely different zone. So, the way this is done that we multiply thermal diffusivity and resolved reaction rate by efficiency function E in order to have the correction in correct turbulent flame speed, so, this E is obtained from the DNS-study.

So, now, the equation would be like that, this is our diffusion and the reaction term on the right hand side, which is modified now with a factor E then thickening by F and the reaction term is multiplied by E/F and this E is flame linking factor or whatever is that efficiency function, which is a strong function of all these parameter like u', S_L, F and δL. So, now by doing that, what we do that that you change. Now there are some advantages some disadvantage with this particular model it solves for individual Y_i that means it.

So, this particular model actually solved for individual mass transfer equation and individual mass transfer equation these diffusivity we can actually at this term actually one can think about this EDd as in like diffusivity D+(E – 1)D. This particular term is correction factor, one can assume that this is your component of the molecular diffusivity and this is the component due to turbulent flux. So, that is why it is consistent with other governing equations.

But the advantage is that it solves for individual species mass transfer equation so, one can now use some sort of an individual kinetics, but in reality, it is not too much of digital kinetics. It has been used in this kind of modelling framework that becomes computationally expensive. Secondly, because of this thickening and all these things, the minor species cannot be captured very nicely.

So, this is one of the drawbacks, and there are lot of these different modifications to these wrinkling factors are proposed and also one can use or look at the dynamical or dynamic variant

of this thickened flame approach or dynamically modified this thicken flame approach. So, these are some of the latest situation of these particular modelling and one can look at the literature to find the latest situation.

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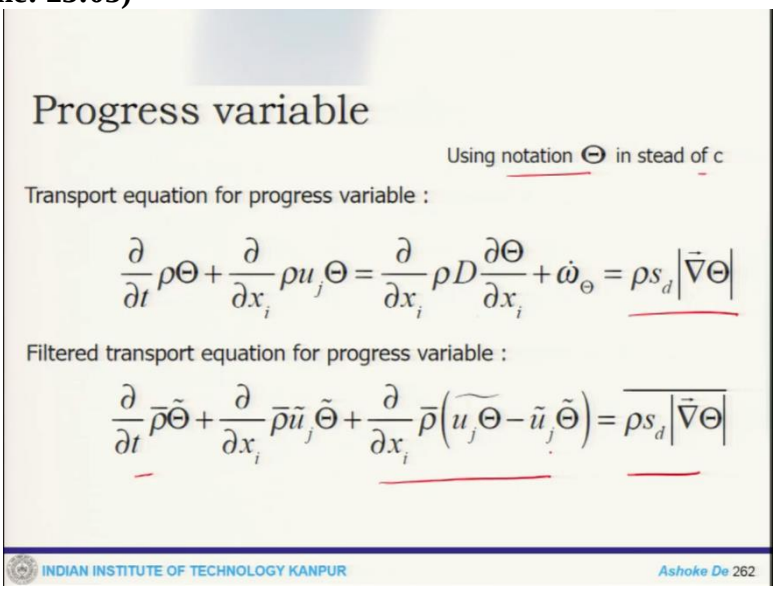

Now, moving to the progress variable kind of approach, where we can use a different notation like this instead of c. So there also, we will use 2 transport equation for this particular progress variable one transport equation for the mean progress variable, like unsteady convection, diffusion and source term, and this is model as ρS_d and once we use the filtered equation, then we get this and there would be which is also model as right hand side is $S_d\nabla\theta$. So, there are terms which are unclosed and one has to do that.

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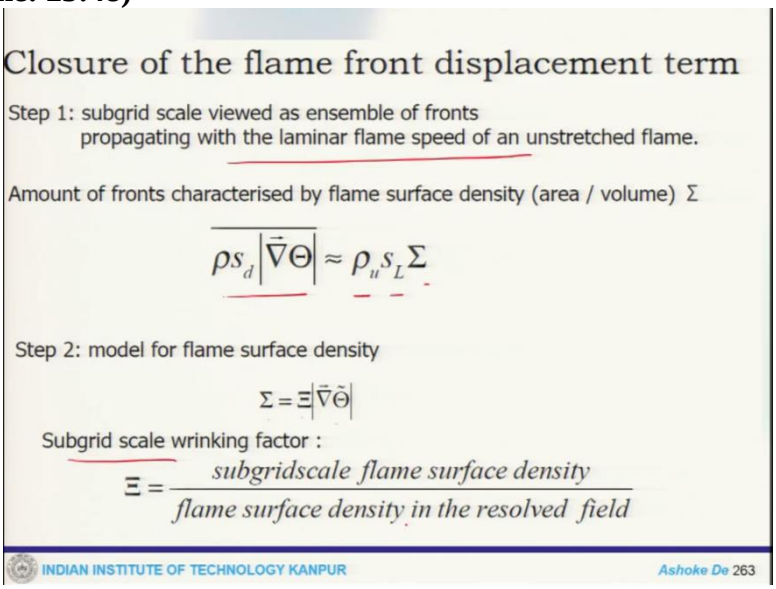

Now, closure for this displacement term. So, the sub grid scale can be used ensemble of fronts propagating with laminar flame speed of an unstretched flame. So, the amount of the flame fronts characterised by the flame surface density is that $\rho S_d \nabla\theta$ would be equivalent to $\rho_u S_L \Gamma$ and surface density. Now we can model for the surface density which is this factor into $\nabla\theta$, this is called subgrid scale wrinkling factor, where subgrid scale flame front density by the density in the resolved field.

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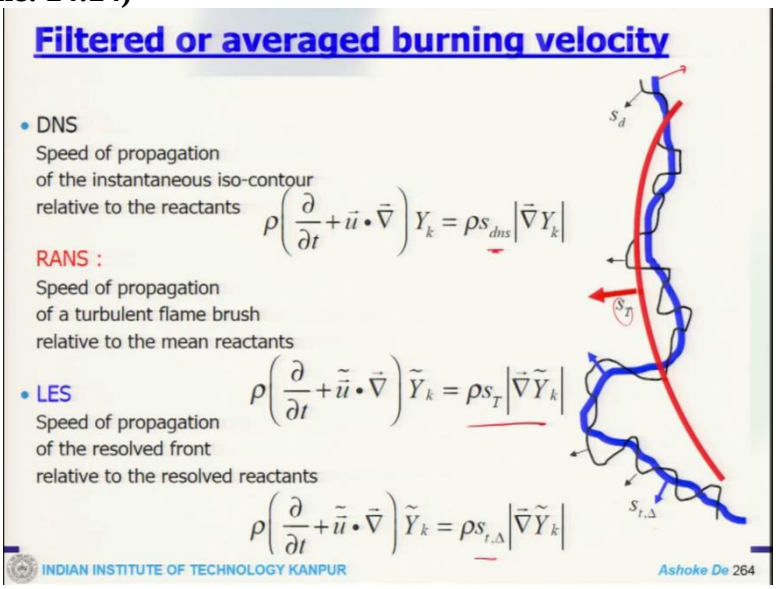

So, this is now, one can use this filtered or averaged burning velocity, which either in DNS situation you get this. This is an instantaneous flame front, this is the mean flame front, where this is your turbulent flame velocity, there is displacement speed and this is the sub grid still stress. Now RANS the speed propagation is relative to the mean. On LES this is to the result reactants and one can correlate from these and use those expression and we have already seen there are different kind of correlations which are available and for more of these, you can.

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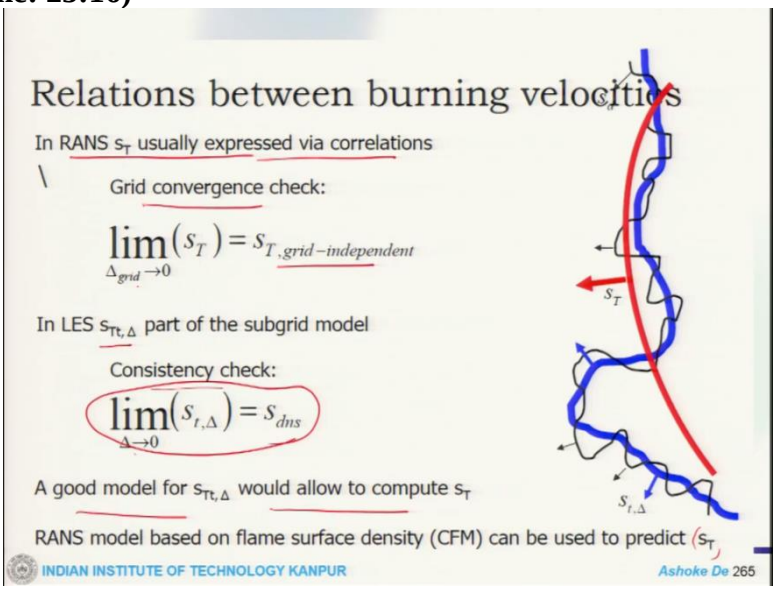

So, the relationship between this is that in RANS, S_T usually expressed by a correlation in the RANS constant and when you look at the grid convergence checks so in the grid convergence checks 0 this would be grid independent. That is but in LES, $S_{T,\Delta}$ is a part of the sub grid scale. So, consistency check is that when Δ tends to do is should goes to DNS. So, that is where it is important. So, that means, they are consistent in nature, so, that you can use this.

So, a good model for $S_{T,\Delta}$ would allow to compute the S_T RANS model based on flame surface density can be used to predict also S_T. So, the one thing is that there are different kind of closure which are available to model one of the other flame, I mean, flame speed, burning velocity and all these things.

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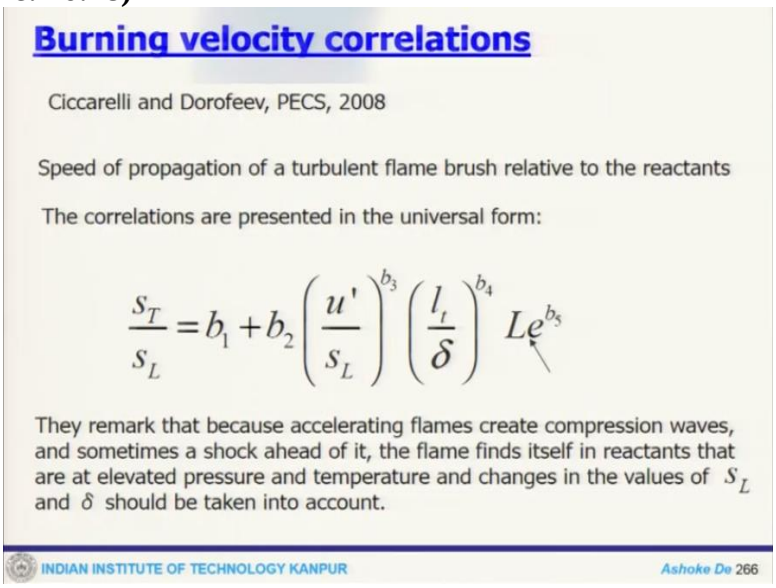

And as we have seen more details of these burning velocities, one can find out this review paper in progress in energy and combustion science, which typically publishes the paper or the review paper on that particular field, where you can see their comparison or collection of different correlations they are all the advantages, disadvantages and all these things.

So, one of the correlations which is in universal form can be used is that S_T/S_L is:

$$\frac{s_T}{s_L} = b_1 + b_2 \left(\frac{u'}{s_L}\right)^{b_3} \left(\frac{l_t}{\delta}\right)^{b_4} Le^{b_5}$$

Now because accelerating flames create compression waves and sometimes a shock ahead of it, the flame finds itself in reactants that are at elevated pressure and temperature change in the values of S_L were taken into account. So, this is the whole idea that one has to take into account.

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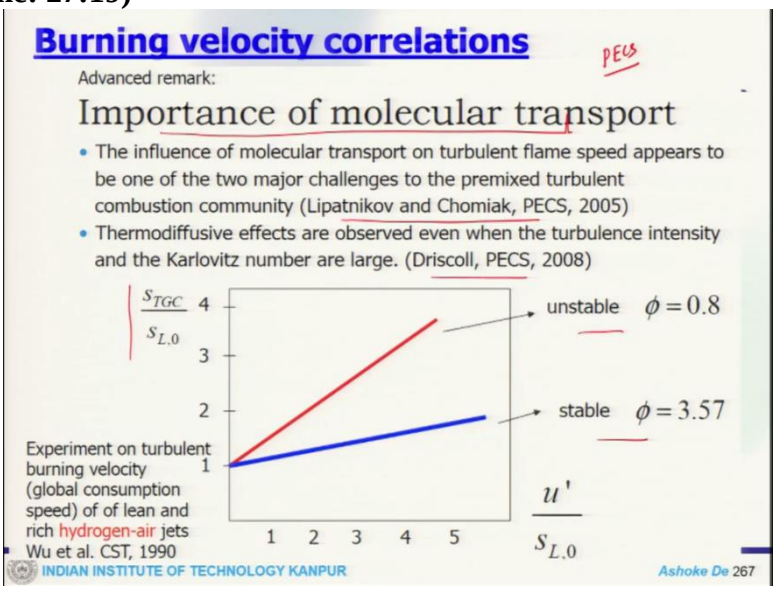

Now slightly more advanced remark, which is that importance of the molecular transport, which says that the influence of molecular transport on turbulence flame speed appear to be one of the two major challenges to premixed turbulent combustion community. So, again these things are detail discussed in these review paper by progress in energy and combustion science in 2005.

And Thermodiffusive effects are observed even when the turbulence intensity and the Karlovitz numbers are large, this is in another paper by Driscoll in 2008. So, where it shows that this ratio with the u primary cell and for difference equivalence issue that becomes unstable. So, these are the advanced remarks and advanced topics or advanced issues, which one can find in

this particular review kind of journal where you can see a lot of review paper which come across.

So that pretty much closed down the discussion on our premixed flame. Now, we will stop it today and continue the discussion on non-premixed flame in the next class.