Turbulent Combustion: Theory and Modelling
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Lecture - 50
Turbulence- Chemistry Interaction (Contd.,)

Welcome back. So let us continue the discussion of this flame speed in the laminar premixed flame so we have looked at the premixed flame diagram and then how different diagram the length scale changes so now this is where we looked at the flame front.

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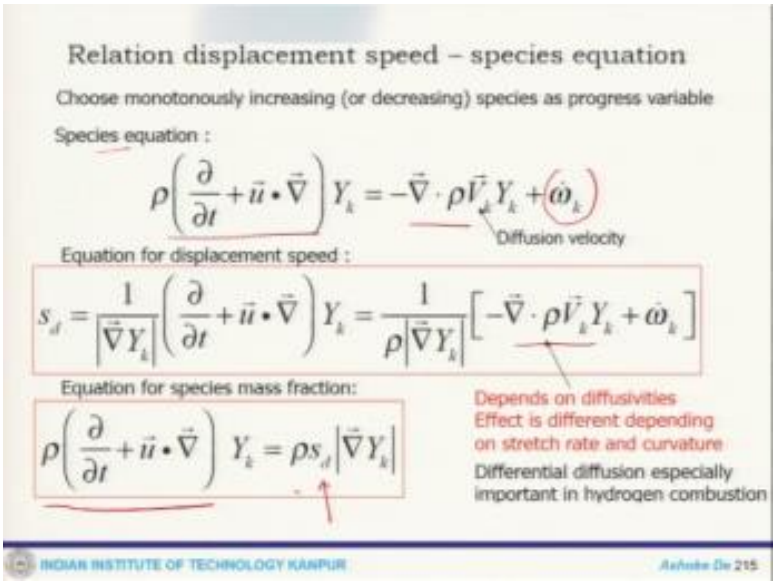

This is at a time instant and there are 2 more information one has to find out is the absolute speed which is $\vec{w}.\vec{n}$. Another is the displacement speed that means how this flame front displaces, so this is what you get? Now one can find out the relation between the displacement speeds in the species equation. Now for our species mass transfer equation, we will write like this and then this is the diffusion part and this is the reaction source term. Now our equation for the displacement speed one can write that $\frac{1}{|\vec{\nabla}Y_k|}$.

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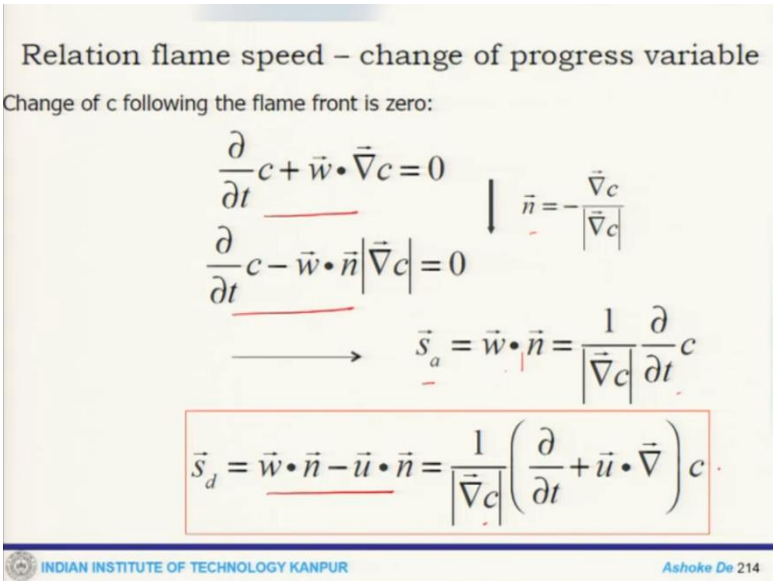

This you know, this particular term depends on diffusivities. So effect of different, effect is different depending on the stretch rate and curvature and one important thing is that that the differential diffusion now become quite important in hydrogen combustion that because hydrogen has a fast mass diffusivity or higher mass diffusivity so that is where that unique Lewis number assumption may not work well.

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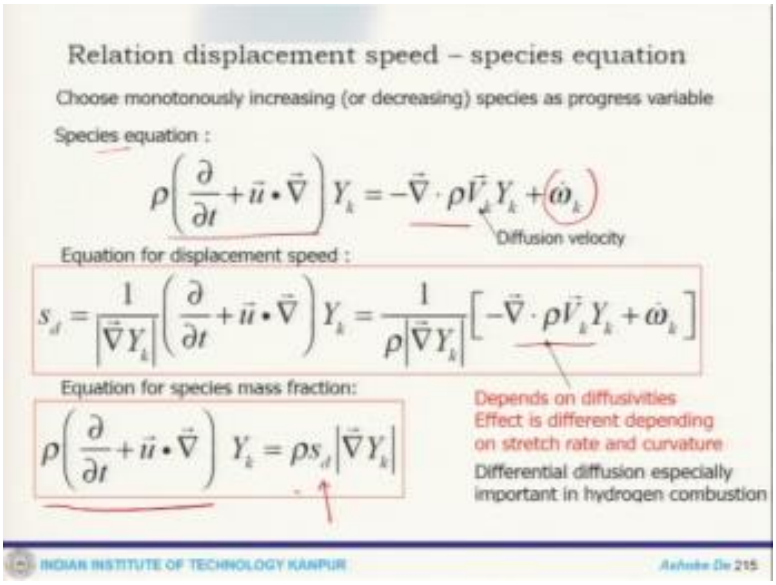

So one has to be careful what kind of fuel is dealing with or rather what kind of flame is dealing with and whether that is quite applicable to the particular situation or not, so now equation of the species mass fraction, so that will now become this is the left hand side or the total

derivative of that and right hand side one can express like $\rho s_d \vec{\nabla} Y_k$, s_d is our displacement speed.

This is the displacement speed and the magnitude of the species mass fraction variance. So now we can see how turbulent burning velocity actually in flamelet regime.

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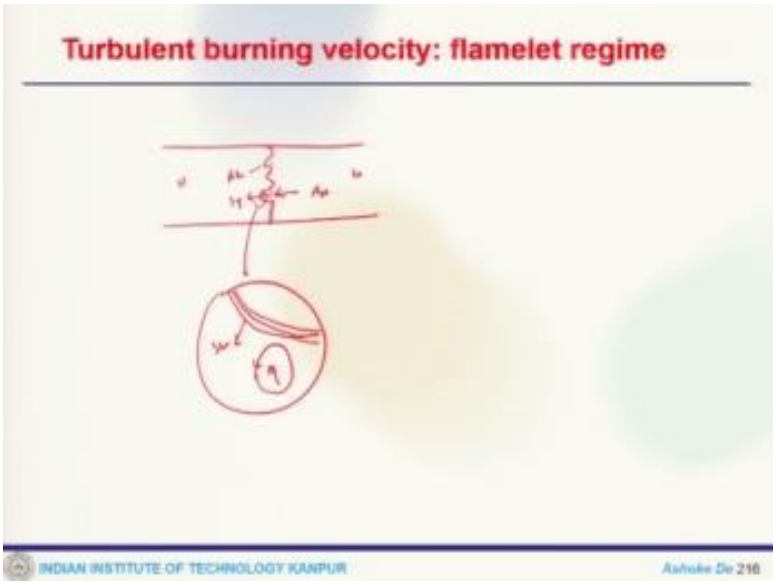

So we take that simple example of that where we get an wrinkle Flamelet like this, so this area one can call it A_M this is A_L and this would be a S_T. This is unburnt side, this is burnt side and particularly this portion if one has to look at so one can think of there is a different smaller layer like this or this would be the S_L and there will be eddy of that scale so low intensity large scale now turbulent flame speed is important.

So which we have already seen that a different correlations exist so which actually now from this volume we can equal the consumption rate of the unburned mixture to that.

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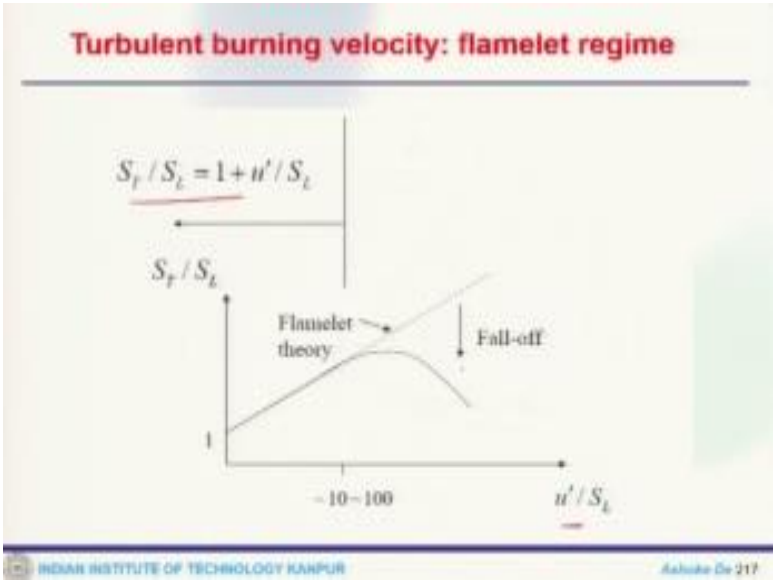

So through which we can get in the Flamelet regime. This is the expression which works which I have already seen and this is the, if you plot that $^{u'}/_{S_L}$ to $^{S_T}/_{S_L}$. This is what the Flamelet theory gives but realistically it goes like that. So there is a deviation from that thing.

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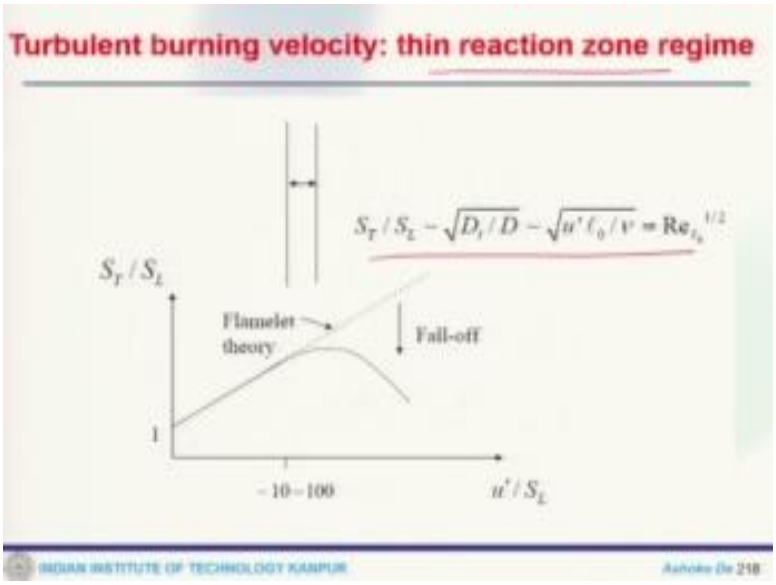

Similarly if we go to thin reaction zone regime this is our theory says that it would be $Re_{l_0}^{1/2}$ and this is how the theory goes but there is a deviation, so though already we have seen there are different kind of expression which are available, but when you actually apply to the system they can vary.

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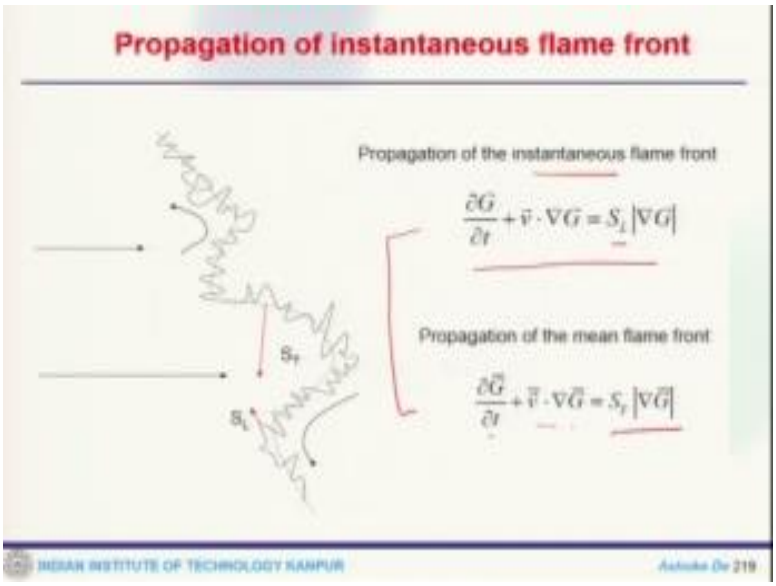

There is another wrinkle Flamelet where you can this is S_L and this is the S_T, so one can find out the capturing of the instantaneous flame front. So this is another very attractive technique for premixed flame front that we capture the instantaneous flame front by an iso surface or other solvarian equation. We will see how that is done that capture that instantaneous flame front to get that thing.

So instantaneous flame front that will propagate and this is called the G is the iso surface which is essentially a distance function. We will see the details when you talk about the G equation and this is how the instantaneous flame front will propagate and if you look at the mean flame front, so $\frac{\partial \bar{G}}{\partial t} + \vec{\bar{v}}.\nabla \bar{G}$ and this would be at the turbulent. So this is our main flame front.

This is our instantaneous flame front. So these two equations are slightly different because when you look at the instantaneous flame front that right hand side you have S_L the mean one propagates with a turbulent flame speed, so when you take into consideration all of this into the equation system and solution for the computational approaches.

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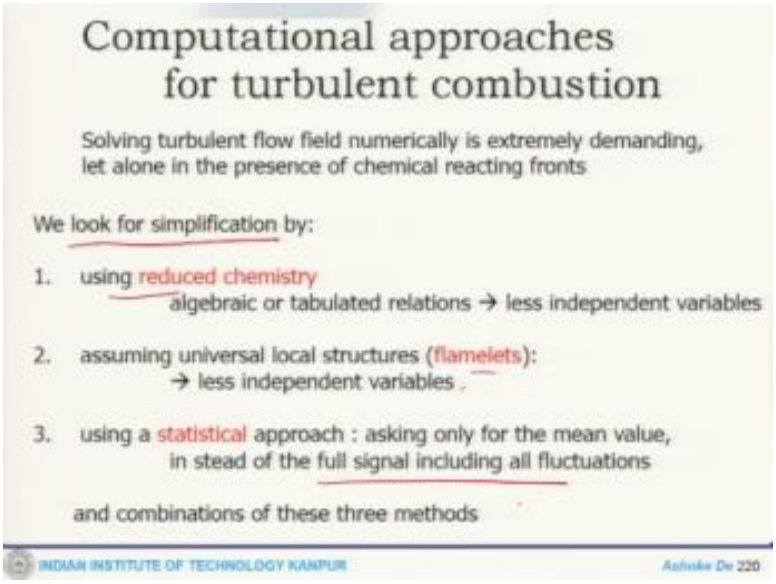

So we have to actually solve this in a quick turnaround time with chemical reactions so one can look for simplifications and what kind of simplifications which are possible you can have reduced chemistry that means you use either algebraic or tabulated reactions, so less independent variable or you can assume the Flamelet kind of assumption local universal structure, so that is also less independent variable or one may use statistical approach and then include the other fluctuations or combination of something like this.

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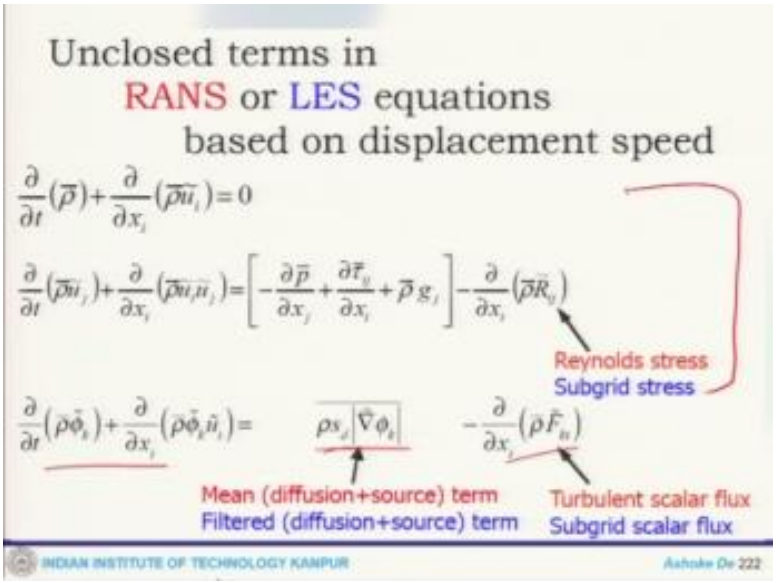

So now when you again go back to the governing equations, whether it is a RANS based and when you look at this equation, these are again density weighted your continuity equation and then momentum equation scalar transport equation so there would be terms like Reynold stress

or Subgrid stress Reynold stress, which is so these RANS the color corresponds to the RANS framework or LES framework.

This would be sub listed on it is RANS framework mean source term or it is a LES it is a filter source term when you go to turbulence scalar flux in RANS it is a subgrid scalar flux, so the equation system when you do RANS or LES filter. They apparently look similar but the terms which you get the closure of those terms would be different because like this in momentum this is the Reynolds stress term, which is using Boussinesq hypothesis one can close it or using different kind of turbulence model but here it says our mistake.

So it requires a different kind of closure, similarly for source term here and subgrid scalar flux also. Now if you use the displacement speed into this governing equation, so these 2 set of equations want change but when you come to the scalar transport equation, so this is in a RANS framework. This would be mean term which is based on diffusion plus source term or in LES is a filtered so that would be again diffusion plus source term and the last term which will remain is turbulence scalar flux which one has to physically close it whether it is in RANS framework or LES framework.

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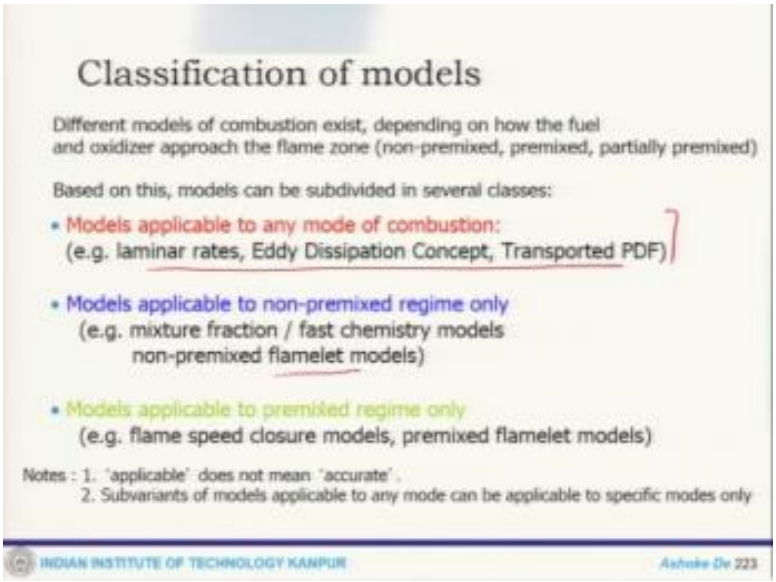

Now, one can classify these models, so the classifications already we have seen the modes of applicant into any mode which is laminar Eddy this is already seen it models which are applicable mixture fraction fast chemistry base model or non premixed combustion on these things.

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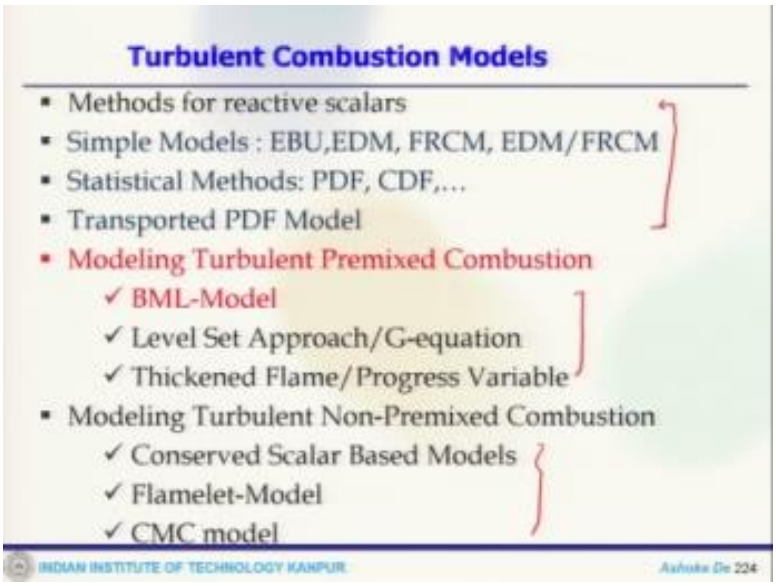

So that is what we talked about these things which is applicable to any mode of combustion. These are very specific to the premixed combustion and these are specific to the non premixed combustion so now we will talk about one start with the BML model which is known as Bray-Moss-Libby model.

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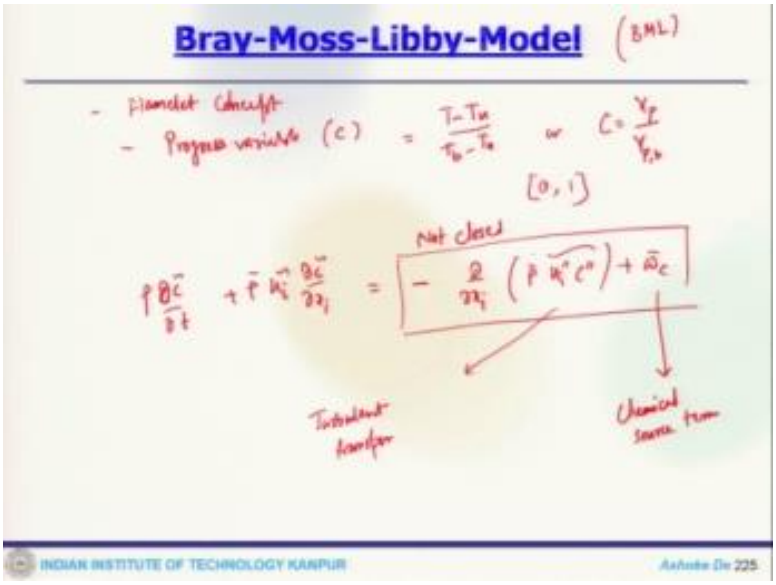

Which is one of the popular model which is a I mean initial days, which was proposed by the scientist and so the concept which is used here is the Flamelet, so that is the concept behind this kind of model in the BML model, so here we solve for a progress variable which is known as c. So either c is defined like in terms of temperature as:

$$c = \frac{T - T_u}{T_b - T_u}$$

Or c can be defined in terms of product mass fraction, which is like this. So it scales between 0 to 1, now the Favre averaged transport equation when you neglect the molecular transport, what we will get:

$$\rho \frac{\partial \tilde{c}}{\partial t} + \bar{\rho}\tilde{u}_i \frac{\partial \tilde{c}}{\partial x_i} = -\frac{\partial}{\partial x_i}\left(\bar{\rho}\widetilde{u_i'' c''}\right) + \bar{\omega}_c$$

So these two terms on the right hand side as we can see they are not closes term, so one need closure for that, now this is the turbulent transport or turbulent flux and this is the chemical source term. So you get these set of equations.

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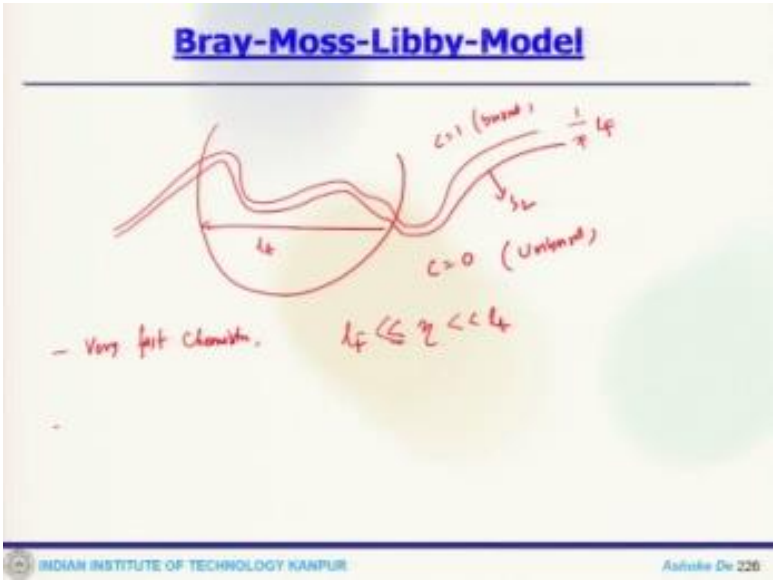

Now you defined a flame front like this, then this is an Eddy size of l_t then this would be S_L and this side it is unburnt, so c is 0 this is unburnt and the side c is 1, which is burnt side, so the assumption which remain there is very fast chemistry that means the flame size this is the l_f the flame size l_f is less than l_t and less than η also. Now another thing is that fuel conversion only in the area of the thin flame front so that could be in the flow field burnt mixture or unburnt mixture or intermediate states are very unlikely.

So that is another assumption which is there you can define a flame front. So in this thin flame front, only the fuel conversion actually takes place.

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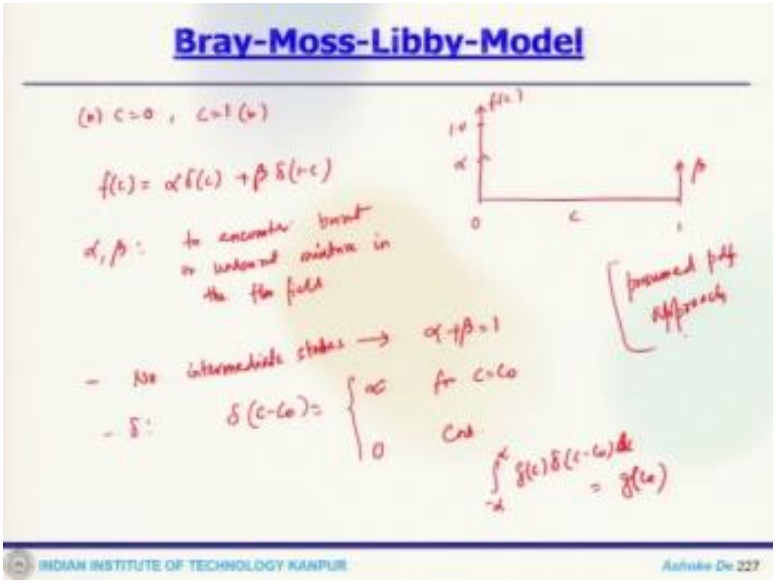

Now what we say that that progress variable would be 0 and 1 this is a case which is unburnt this is a case which is burnt this is solely expected to behave between 0 and 1 so the probability density function f(c) would be:

$$f(c) = \alpha\delta(c) + \beta\delta(1 - c)$$

So if you put that thin. This is 0 this is 1 this is β and this is how you get α if c is 1 this is c. So this α and β these are the probabilities to encounters or to encounter burnt or unburnt mixture in the flow field.

So there is no intermediate states which means $\alpha + \beta$ would be 1 and then δ function which is defined as $\delta(c - c_0)$ which could be infinity for c equals to c_0 or 0 for constant which gives:

$$\int_{-\infty}^{\infty} \delta(c)\delta(c - c_0)\, dc = g(c_0)$$

So this is how we define this but one thing here this probability distribution function the definition here is that this functions are applied. We assumed or presumed that is why this flamelet kind of approach is also known as presumed PDF approach. Okay? But what did we discuss which is in hybrid combination like lagrangian and ordinance that said transported PDF approach where you have a transport equation for the probability distribution function here. We solve for a different transport equation, but assuming the distribution with apriori shape of that PDF and that is why it is known as presumed PDF method.

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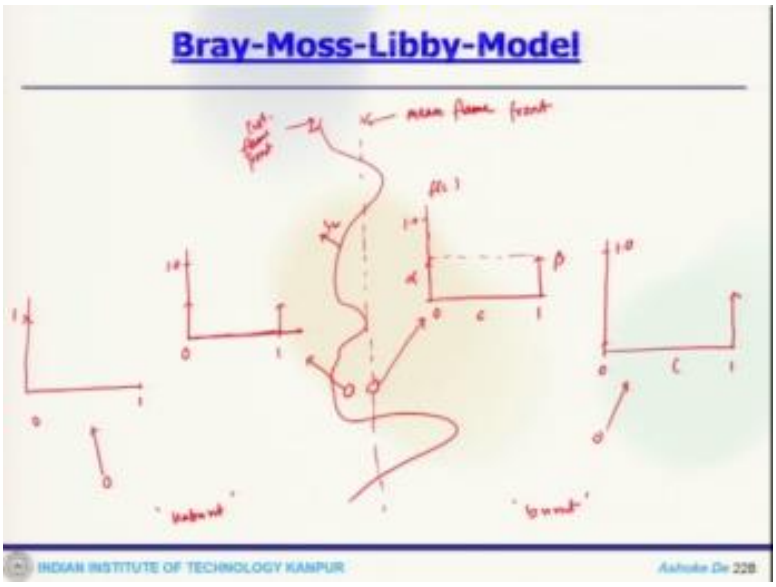

So now if your instantaneous flame front go like this then I can draw some line here where you can have this one position like this is my mean flame front, this is how my S_L is going to behave. This is an instantaneous flame front and this side is unburnt obviously and this side would be burnt so there could be one state here and there could be one state there. Now this state if you look at the c, this will go between 1 and 0.

So this is how it behaves, so that means this would be completely 1 now if I look at this stage where it goes between 1 and 0, so this is what it is and this is 1, here along the mean flame front position you can define that this is $\beta_1 c_0 \alpha$ and somewhere 1 that is rfc. So you can have these which is 0, c goes to 1, so you goes like that it goes like that, and that is i.

So you can see that when you look at the instantaneous flame front at different situation this is completely at the unburnt state and how this function is behaving the product distribution function. This is somewhere within the reaction zone is at the mean flame front. This is at the burnt state completely.

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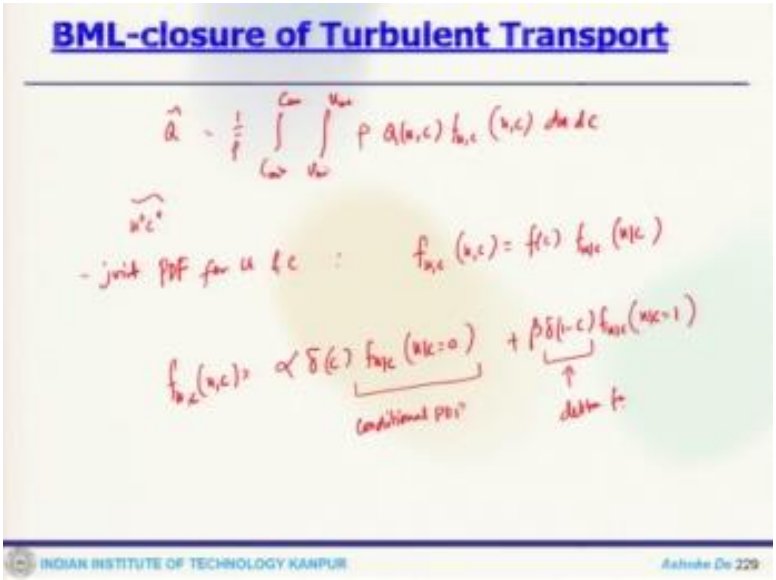

Now we can use favre filtering for favre averaging. One can write this is:

$$\tilde{Q} = \frac{1}{\bar{\rho}} \int_{C_{min}}^{C_{max}} \int_{u_{min}}^{u_{max}} \rho Q(u,c) f_{u,c}(u,c) du dc$$

Now therefore the unclosed term we can correlate like using the, this is the unclosed term which we can correlate this $\widetilde{u''c''}$ using either joint PDF for u and c which is:

$$f_{u,c}(u,c) = f(c) f_{u/c}(u/c)$$

Which is the Bayes theorem or introducing the BML approach for:

$$f_{u,c}(u,c) = \alpha\delta(c) f_{u/c}\left(\frac{u}{c} = 0\right)$$

So this is an conditional PDF and we also got :

$$\beta\delta(1-c) f_{u/c}\left(\frac{u}{c} = 1\right)$$

And this is our delta function. So this is what you can close or write using BML.

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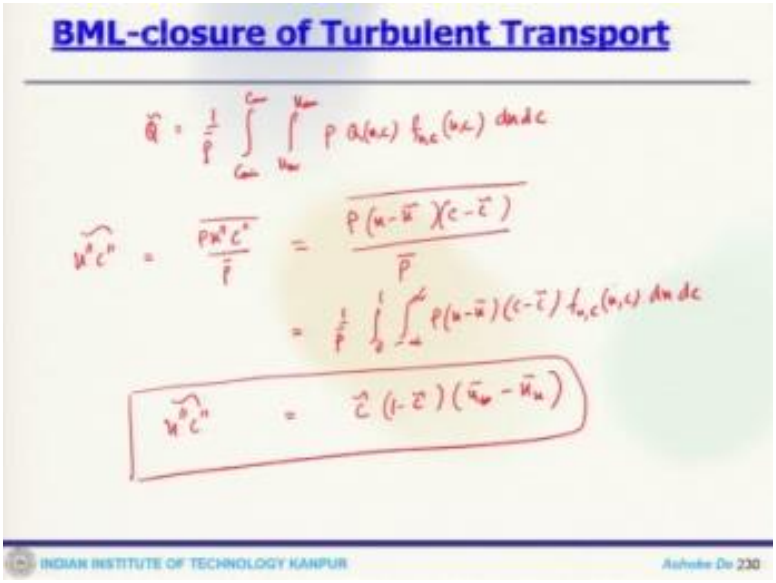

So now this quantity you can write:

$$\tilde{Q} = \frac{1}{\bar{\rho}} \int_{C_{min}}^{C_{max}} \int_{u_{min}}^{u_{max}} \rho Q(u,c) f_{u,c}(u,c) du dc$$

You allow to close this as:

$$\widetilde{u''c''} = \frac{\overline{\rho u''c''}}{\bar{\rho}}$$

Which is:

$$\widetilde{u''c''} = \frac{\overline{\rho(u-\tilde{u})(c-\tilde{c})}}{\bar{\rho}}$$

Which is:

$$\widetilde{u''c''} = \frac{1}{\bar{\rho}} \int_0^1 \int_{-\infty}^{\infty} \rho(u-\tilde{u})(c-\tilde{c}) f_{u,c}(u,c) du dc$$

Which will give you finally that:

$$\widetilde{u''c''} = \tilde{c}(1-\tilde{c})(\overline{u_b} - \overline{u_u})$$

So this is a closure for that term using this BML approach you get this simplified expression, which can be used.

Now another thing is that one can use the counter gradient diffusion. So let us say.

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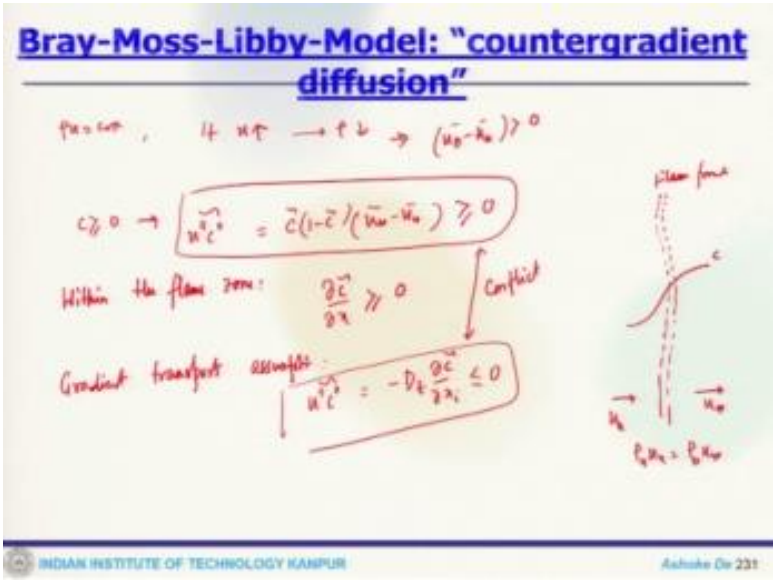

If we have a flame front like that which is u_u, u_b, ρ_u, and ρ_b. This is c and this is my flame front, now since ρ_u equals to constant through flame front I mean ρ_u constant through flame front if u increases so ρ decreases that means my u_b - u_u would be positive now because c greater than equals to 0. So this term I can write:

$$\tilde{c}(1-\tilde{c})(\overline{u_u}-\overline{u_b}) \geq 0$$

Now this is in flame front within the flame zone. If you look at it $\frac{\partial \bar{c}}{\partial x}$ which is greater than 0. Now if I use our gradient transport assumption, I can write:

$$\widetilde{u''c''} = -D\frac{\partial \bar{c}}{\partial x} \leq 0$$

So there is a conflict with the counter gradient diffusion in BML model.

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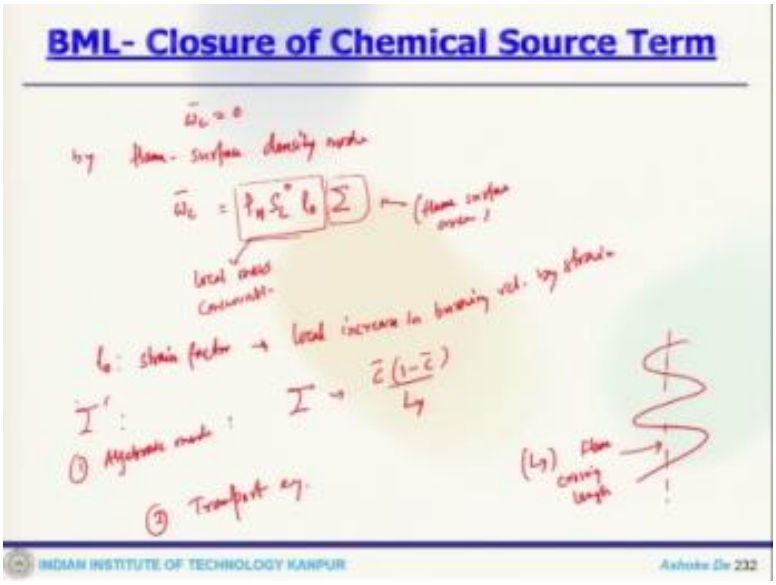

Now chemical source term we can using our f_c leads to that w_c is 0. Now that is why we close it by flame surface density model or w_c is written as $\rho_u S_L^0 l_0 \Gamma$. So this is quantum this is another term this is our local mass conservation this is flame surface area per volume l_0 is our strain factor which actually, so the strain factor. So there is always a local increase in burning velocity by strain now the flame surface density Γ there is an algebraic model I mean there could be so this is a local mass conservation.

So if you let us say I have a flame font like this I mean this is our mean let us say this is our flame crossing length which let us say L_y then the film surface density. We need a closure because this term in the source term is the local mass conservation so which is available and this is another term which is required so 1 option is that one can use algebraic model which is closing this term as $\frac{\bar{c}(1-\bar{c})}{L_y}$.

So this is a simple expression one can use for this or one can use the transport equation. So that is another option one can use to closure this model.

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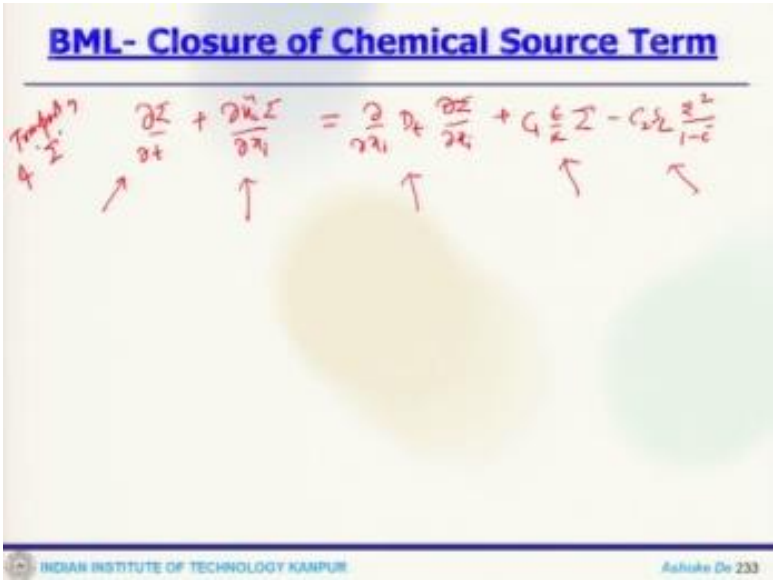

So the transport equation would be in terms of Γ one can write:

$$\frac{\partial \Gamma}{\partial t} + \frac{\partial \tilde{u}_i \Gamma}{\partial x_i} = \frac{\partial}{\partial x_i} D_t \frac{\partial \Gamma}{\partial x_i} + C_1 \frac{\epsilon}{K} \Gamma - C_2 S_L \frac{\epsilon^2}{1-\bar{c}}$$

So this is our local change, this is convective change of the flame surface, this is the transport equation. This is turbulent transport, this is production due to stretching of the flame and this is flame and illusion.

So when you look at this transport equation, this is transport equation of r flame surface density, so the left hand side looks like any other transport equation. Then right hand side you have the diffusivity production term due to flame state and the other terms and the detailed analysis we will continue in the next lecture. So we will stop here today.