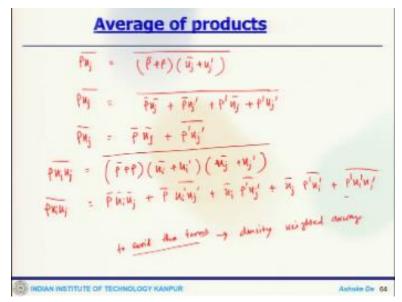
Turbulent Combustion: Theory and Modelling Prof. Ashoke De Department of Aerospace Engineering Indian Institute of Technology - Kanpur

Lecture-44 Turbulence - Chemistry Interaction (Contd.,)

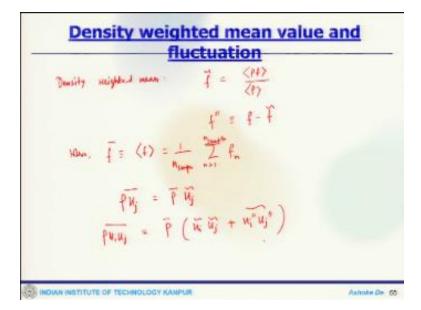
Welcome back and let us continue the discussion of this averaged equation in transfer mode.

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So we are looking at this average of the product and this is what we looked at when you take this, $\overline{\rho u_j}$ and $\overline{\rho u_l u_j}$ and we can see some terms contribute to density, fluctuation. So if you keep those things that would create suffering. So the idea is that to avoid these terms, so that is what we go for density-weighted average.

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So how you do that now density-weighted average, let us say density-weighted mean if we say then f would be sometimes we call it also Favre averaged. Okay, then the fluctuation related to the density-weighted mean would be a f'' which is

$$f'' = f - \tilde{f}$$

where \tilde{f} is $\langle f \rangle$, which is ensemble average of this is n samples summation over 1 to samples F n, now what it allows you that it allows you to that now

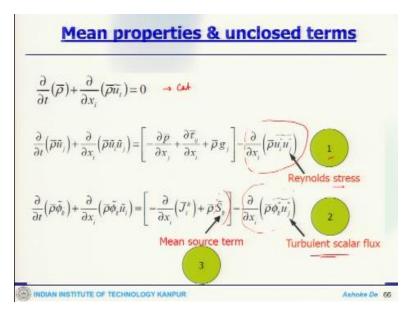
$$\overline{\rho u_j} = \bar{\rho} \, \widetilde{u_j}$$

and $\overline{\rho u_l u_l}$ that will become

$$\overline{\rho u_i u_j} = \bar{\rho}(\widetilde{u_i}\widetilde{u_j} + \widetilde{u_i'' u_j''})$$

so you can avoid the term which is like density, fluctuations in these terms. So that is one of the advantages when you have a reacting system. It is a good idea to go for density-weighted average or we call it also Favre average.

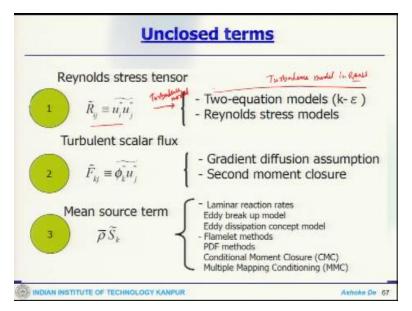
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Now we can see this mean property and the terms. So the whole idea is that now my governing equation would be again based on this Reynolds averaging or Fevre averaging or density-weighted averaging the set of governing equations would be now again transformed. So, once we do that, this is my continuity equation. Now instead of \bar{u} this would be using the momentum equation will get back an extra term, which is called the Reynolds stress term and my scalar transport equation.

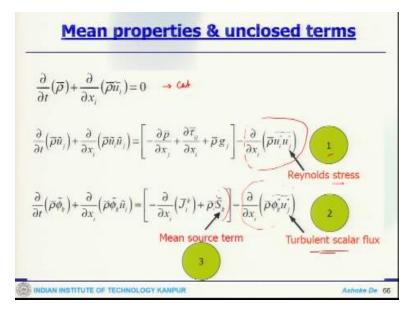
We will have one term which is a mean source term this could be a source term due to chemical reaction. This could be anything and there will be an additional term which is called the turbulence scalar flux. So these 3 terms in terms like term 1 Reynolds stress, term 2 turbulence scalar flux. terms 3 the mean Source term, if you look at the complete governing equation, these 3 terms are not actually closure term. So we need some sort of a closure approximation for this term and this is one of the challenging ways one encounter while closing this term.

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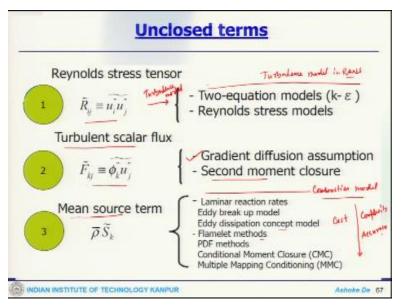
Now we can see and correlate how so now when you try to close this Reynolds stress term, this is where you need to invoke your turbulence model. So your turbulence model will allow you to so either you can use a different kind of RANS model LES model or whatever it is. So it is a variant of the turbulence model in the RANS framework, so we are not talking about anything on LES because the equation system would look different, so that is what we know.

So any RANS based equation like 2 equation model Standard k-ε turbulence model, k-omega model or RSM that would close down this and how and it will only deep rise to your edification and all these things that we have already seen as a part of our discussion in turbulence model. Now, this is why the importance of turbulence modeling or the discussion on turbulence was required. (**Refer Slide Time: 05:14**)



Because now this should be much easier to see when this enclosed term actually appears in the governing equation how we close it now, the second term is turbulence scalar flux, so which is written in this fashion. So typically we use the gradient diffusion assumption though it is widely accepted in only a few specific cases this may lead to some spurious results or one may use second-moment closure. Now, that means source term that is what is the point of interest that is the chemical source term.

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Now you require all short of turbulence chemistry interaction model or one can call it in. All range of this is combustion model, so you need these models which will allow you to close down that mean source term. So it could be laminar reaction rate, Eddy breakup model, EDC model, flamelet

method, PDF method, CMC or MMC the so this is with the order of increasing expenses in the sense competition expenses at the same time the complexity also so this increases the complexity.

So at the same time cost but at the same time, it increases quite a bit of accuracy also. So all these things increase as you go from top to bottom.

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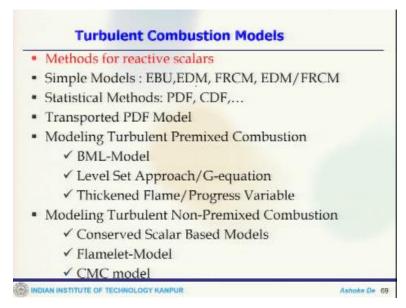
| Different models of combustion exist, depending on how the fue and oxidizer approach the flame zone (non-premixed, premixed | |
|--|-------------------------|
| Based on this, models can be subdivided in several classes: | |
| Models applicable to any mode of combustion: (e.g. laminar rates, Eddy Dissipation Concept, Transport | ted PDF) |
| Models applicable to non-premixed regime only (e.g. mixture fraction / fast chemistry models non-premixed flamelet models), CHC, NHC | |
| Models applicable to premixed regime only (e.g. flame speed closure models, premixed flamelet models) | nodels), <mark>c</mark> |
| Notes : 1. 'applicable' does not mean 'accurate'. 2. Subvariants of models applicable to any mode can be applicable | to specific modes only |

Now the different models which one may like to use for what we are talking about this kind of combustion. So the models which are applicable to any mode of combustion could be laminar finite rate kind of model, EDC kind of model, or transported PDF kind of model. So theoretically when we look at the theoretical description, these models ideally can be adapted for any kind of mode of combustion whether it is premixed, non-premixed, or partially premixed.

Now some models are applicable to non-premixed regime only that is mixer fraction or fast chemistry model then the flamelet based model, CMC, MMC. These are primarily used for the non-premixed regime rather they are quite good enough for this regime. When you move to the premixes, it requires a lot of theoretical modification and which is applicable to premix them which is a flame surface closure model or flame speed closure model is premixed flamelet model G equation models and other models like that.

So there are essentially you try to I mean sort of that capture the flame topology and this now when you say the applicability that does not mean the accuracy so there are some variants of models applicable to any mode can be applied to specific modes only. So this is what one has to be very careful when talking about these combustion models because they can be applied to anywhere, but that does not mean this will provide you accurate results.

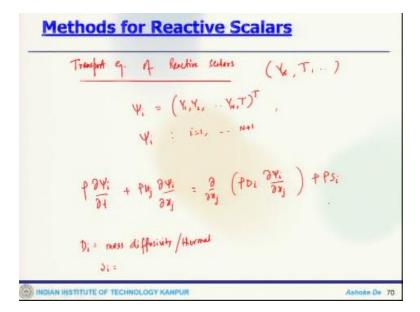
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Now, what we will do now, these are the set of models that one can see there are simple models.

There are statistical based models transport PDF models, then the models which are very specific to premixed combustion. There are model which is specific to non-premixed combustion. So this should give you an idea of how we are going to span our discussion around this. Okay. So first we start with the method of reactive scalars.

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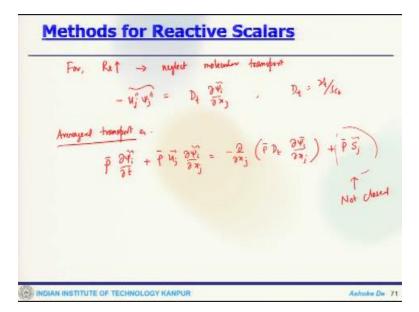
So you have a transport equation of any reactive scalars, so the reactive scalars could be species mass fraction. Let us say Y_{α} or Y_i and they could be temperature like that. Now I can put that thing in a functional form, which is Y_1 , Y_2 to Y_n and temperature, so the balanced equation where this ψ_i which goes for i equals to 1 to N + 1 because of N number of species and then temperature.

So the balanced equation would look like

$$\rho \frac{\partial \psi_i}{\partial t} + \rho u_j \frac{\partial \psi_i}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\rho D_i \frac{\partial \psi_i}{\partial x_j} \right) + \rho S_i$$

It is just like another scalar transport equation where D_i is your mass diffusivity and it could be thermal diffusivity and then S_i is the source term whether it could be chemical source term or temperature source term.

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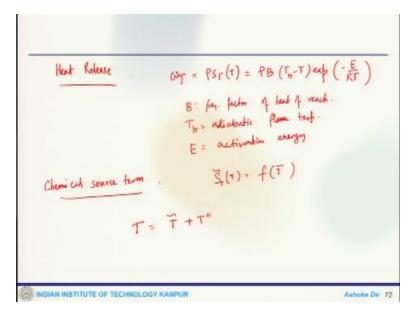
Now for the high Reynolds number, we can neglect the molecular transport so that if we neglect then the gradient transport assumption of the turbulence transport can be used to close this term like u j double prime. So this term we can use the gradient hypothesis and we can close this term where D_t would be v_t/Sc_t then the average transport equation would take the form

$$\bar{\rho}\frac{\partial\widetilde{\psi_{i}}}{\partial t} + \bar{\rho}\overline{u_{j}}\frac{\partial\widetilde{\psi_{i}}}{\partial x_{j}} = -\frac{\partial}{\partial x_{j}}\left(\bar{\rho}D_{i}\frac{\partial\overline{\psi_{i}}}{\partial x_{j}}\right) + \bar{\rho}\widetilde{S}_{j}$$

these are obvious when you talk about average, these are all density-weighted average or have the average.

So again this theorem, still if you see this term, this is not closured. So this requires some closing. So we need to approach like our turbulence models expression for some mean values and something.

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Now we can write our heat release. So the heat released term one can write that

$$\omega_T = \rho S_T(T) = \rho_B(T_B - T) \exp\left(-\frac{E}{RT}\right)$$

Here B is the frequency factor of the heat of reaction T_B is the adiabatic flame temperature and is the activation energy now we need chemical source term, which has to be also closure or require some modeling so that we can say that it is a function of temperature. Now this temperature has been widely accepted we can decompose into 2 components T as T fluctuation.

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$$\begin{split} \hline T_{\text{Ayber expansion}} & T \neq T & (T = T + T^*, T^* \leftarrow T) \\ & \tilde{\varsigma}_{T}(T) = B (T_{V} - T) \exp \left(-\frac{E}{RT}\right) \\ & \tilde{\varsigma}_{T}(T) = B (T_{V} - T) \exp \left(-\frac{E}{RT}\right) \\ & \text{Pre. echoreuslied team:} (T_{V} - T) \Big|_{T = T} \approx T_{V} - T^* - T^* \\ & \text{Expansional team:} -\frac{E}{RT} \approx -\frac{E}{R} \left[\left[\frac{1}{T} - \frac{1}{T_{T}} + \left(T - T\right) \right] \right]_{T+T^*} \\ & = -\frac{E}{RT} + \frac{ET^*}{RT^*} \\ & \tilde{\varsigma}_{T}(T) \Big|_{T = T^*} \approx B (T_{V} - T - T^*) \exp \left(-\frac{E}{RT}\right) \exp \left(\frac{ET^*}{RT^*}\right) \\ & \tilde{\varsigma}_{T}(T) = \frac{1}{T = T^*} = \frac{1}{T} \exp \left(-\frac{1}{T} + \frac{1}{T}\right) \\ & \tilde{\varsigma}_{T}(T) = \frac{1}{T = T^*} = \frac{1}{T} \exp \left(-\frac{1}{T} + \frac{1}{T}\right) \\ & \tilde{\varsigma}_{T}(T) = \frac{1}{T = T^*} = \frac{1}{T} \exp \left(-\frac{1}{T} + \frac{1}{T}\right) \\ & \tilde{\varsigma}_{T}(T) = \frac{1}{T} = \frac{1}{T} = \frac{1}{T} + \frac{1}{T} + \frac{1}{T} + \frac{1}{T} + \frac{1}{T} \\ & \tilde{\varsigma}_{T}(T) = \frac{1}{T} = \frac{1}{T} + \frac{1}{T} +$$

So we can use our Taylor series expansion or Taylor expansion. So if I use Taylor expansion then

$$T \approx \tilde{T} \ (T = \vec{T} + T'', T'' \ll \tilde{T})$$

So then we can write

$$\widetilde{S_T}(T) = B(T_b - T) \exp\left(-\frac{E}{RT}\right)$$

Pre-exponential term:

$$(T_b - T)|_{T = \tilde{T}} \approx T_b - \tilde{T} - T^{\prime\prime}$$

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Now because of Favre mean what we get that this is equivalent to

$$\widetilde{S_T}(T) = B(T_b - T) \exp\left(-\frac{E}{RT}\right)$$

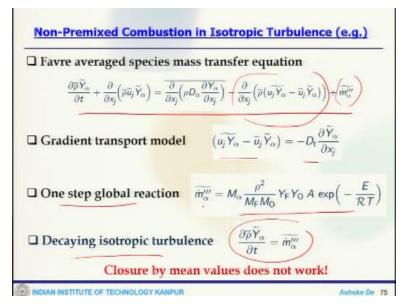
$$\Downarrow$$

$$\widetilde{S_T}(T) = \widetilde{S_T}(\overline{t}) \left(1 - \frac{T''}{T_b - \widetilde{T}}\right) \exp\left(\frac{ET''}{R\widetilde{T}^2}\right)$$

now the typical value this term $\left|\frac{T'}{T}\right|$ actually lies between 0.1 to 0.3. These are some typical values. But not necessarily it is going to be this is in the reaction zone of flame.

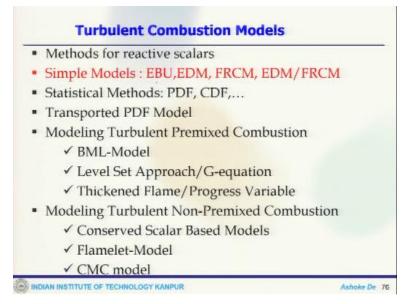
Now if you have intense fluctuation of the chemical source term around the mean value this moment method that we are describing here is quite inappropriate due to the strong nonlinear effect of the chemical source term. So if the fluctuations are too high, this is not quite accurate because of this non-linearity

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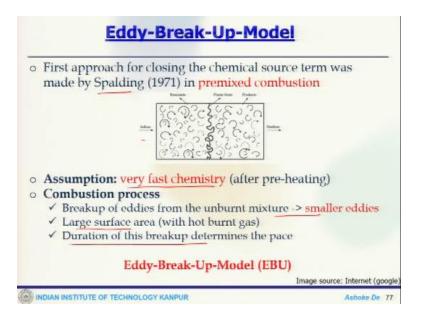
Now we can look at this thing in for example in the isotropic turbulence case. This is how your Favre averaged specialist transport equation looks like. This is the unclosed term. Then this is closed like a radiate transport model if you use a one-step global reaction. So this chemical Source term can be represented like this and if it is decaying isotropic turbulence, then you can write like this. This is just an example. So here, the closure by mean values does not work. So we have to think about something else

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So now we can look at some of these simple models and see how they have derived now the Eddy breakup model it was fast.

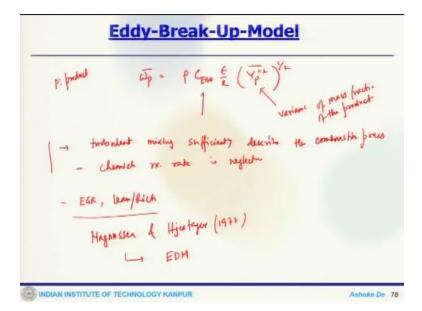
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This is something that is used to close the chemical Source term for in pre-mixed combustion and it was proposed in 1972 by Spalding. So you have the inflow there is a reactant and there is a flame front then the product is an outflow. So there are serving assumption which is sort of associated with this that is one of the important assumptions is the very first chemistry. Soda combustion process what it says that the breakup of Eddie's from the unburnt mixer to the smaller mixer band that means from this side to that side.

So due to this thing large surface area and duration of this breakup determine is the pace. So that is why this whole terminology came up that Eddy breakup model because how the Eddy breaks up depending on that the reaction Source term.

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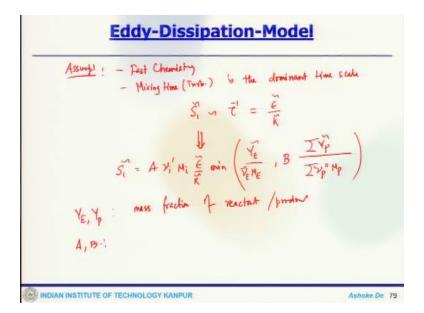
Now, if you look at the average reaction source term for a product. Let us say P stands for the product. Then

$$W_p = \rho C_{EBU} \frac{\varepsilon}{R} (\overline{Y_p^{\prime\prime 2}})^{1/2}$$

 $(\overline{Y_p''}^2)^{1/2}$ is the variance of mass fraction of the product and this is the Eddy Break up model constant now here the 2 things that happens are the turbulent mixing sufficiently describes the combustion process. That is number 1 number 2 chemical reaction rate is neglected or negligible.

So this is quite simple, but there are issues. Like if you want to use for let us say EGR or lean or reach combustion condition. This is not quite applicable. So then this model was further developed by Magnuson and 1977 which is called the EDM Eddy dissipation model. So the first modification was of this Eddy breakup model to EDM.

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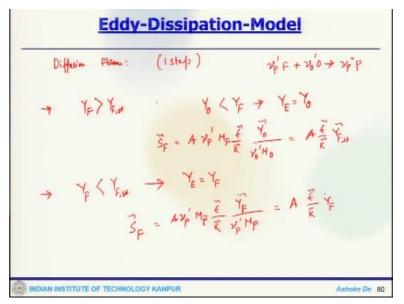


Now what EDM does that also have a certain assumption? So, one of the assumptions is that also fast chemistry. That is a very fast chemistry and mixing time. Mixing time which is turbulent mixing time is the dominant time scale their dominant time scale. So This means that S_i is the order of τ^{-1} , which is ϵ/K . So that will lead to model my chemical source term which can be written as

$$\widetilde{S}_{1} = Av_{1}'\mu_{i}\frac{\vec{\varepsilon}}{\vec{k}}\min\left(\frac{\widetilde{Y_{E}}}{\widetilde{v_{E}}M_{E}}, B \frac{\sum \widetilde{Y_{P}}}{\sum v_{p}''M_{p}}\right)$$

Where Y_E , Y_P these of the mass fraction of the reactant so, mass fraction of reactant and or product A B these are the model parameter. So these are sort of determined.

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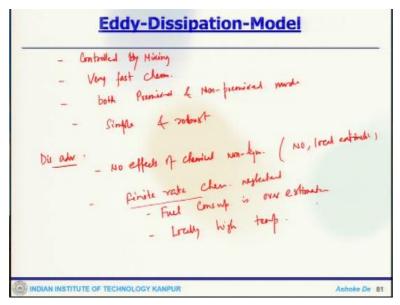
Now if you apply to a diffusion flame, for example, let us say diffusion flame. One Step chemistry where you write fuel plus oxidizer to the product so that kind of one step chemistry if you consider, so you could have let us say Y_F which is greater than Y_F stoichiometric. Then what happens Y oxidizer would be Y_F and that will lead to Y_E is Y oxidizer, so S_F would be written as

$$\widetilde{S_F} = Av'_F M_F \frac{\vec{\varepsilon}}{\vec{k}} \frac{\widetilde{Y_o}}{\widetilde{v_o} M_o} = A \frac{\vec{\varepsilon}}{\vec{k}} \widetilde{Y_{F,st}}$$

the other situation what could be possible that Y_{A} is less than $Y_{\text{F},\text{St}}$ which will lead

$$\widetilde{S_F} = Av'_F M_F \frac{\vec{\varepsilon}}{\vec{k}} \frac{\widetilde{Y_F}}{\widetilde{v_F} M_F} = A \frac{\vec{\varepsilon}}{\vec{k}} Y_F$$

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Now if I put some of these issues so there one can see that it is primarily mixing control phenomena that is number one, very fast chemistry, and the application it can be applied to both. premixed and non-premixed mode Now it connects the turbulent mixing with the chemical reaction, so the reach or lean either full or partial conversion this can be this does not come into consideration. It is simple and robust that is one of that but there are certain disadvantages which are quite prominent.

So no effects of chemical non-equilibrium that is one thing that is that mean that NO formation, local extinction that cannot be predicted. Extinction then also the finite rate chemistry effect is not

finite rate chemistry effect. Chemistry effects are not considered. So, the fuel consumption is overestimated that is number one, then you can have locally high temperature also. So, the finite rate chemistry is neglected so because of that you can have fuel consumption which is overestimated, and locally high temperature.

So, these are some of the issues with the Eddy dissipation model. So, we will look at the other model and how to overcome this particular issue. So, we stop here today and continue the discussion in the next lecture.