Turbulent Combustion: Theory and Modelling
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Lecture - 47
Turbulence- Chemistry Interaction (cont…)

Welcome back, let us continue the discussion on the transport medium model so we what we have looked at the basic definitions and then the governing equations in the Eulerian framework and then we have also discussed about some of the unclosed terms which are sitting there in the transport equation how to close them that is what we are now doing it. Now in order to do that, we have also discussed the different velocity PDF, velocity scalar PDF and also the scalar PDF and then we started looking at the governing equation.

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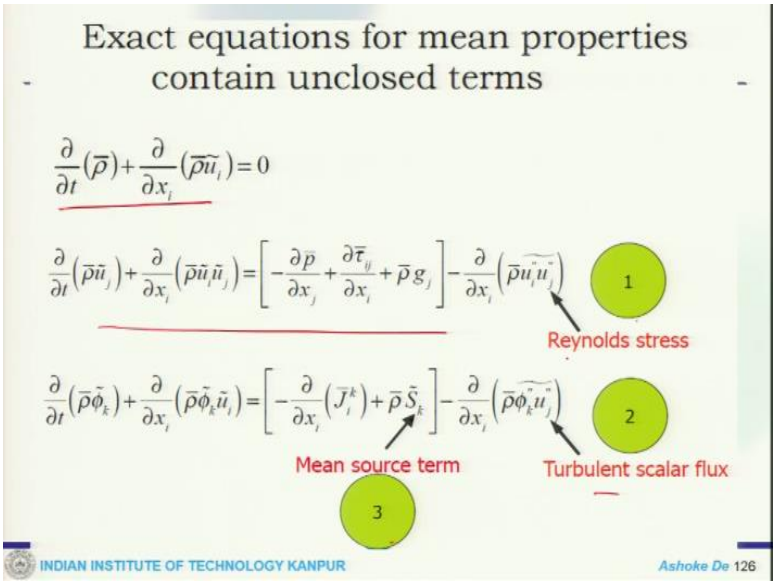

This is what we are up to. So once you look at those things in the averaged equation system. So you get 3 unclose terms number 1, 2, and 3 this is Reynolds stress, turbulent scalar flux means sources term.

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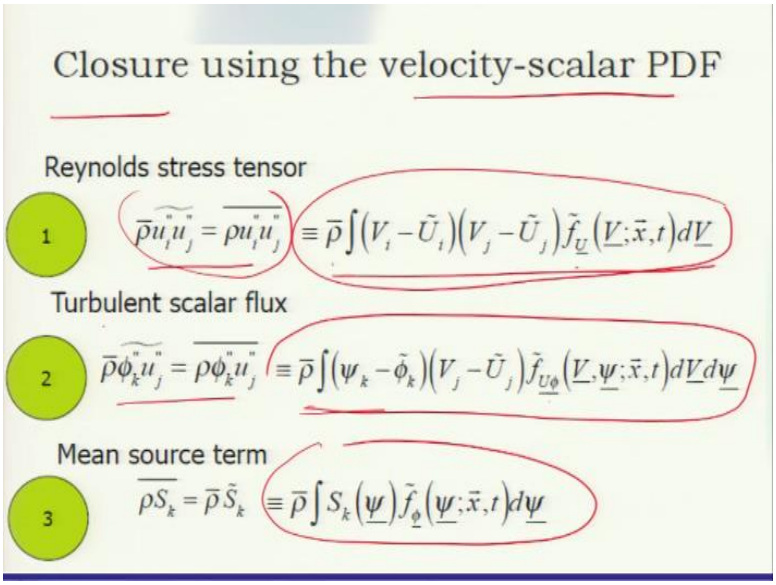

Now when you close them previously, we have already seen that to close that this term we use some turbulence model. So here also if you are only using the scalar PDF approach then use the turbulence model or any RANS model to close it. Scalar flux, we can use the gradient diffusion model and the only reaction Source term we can close it using the scalar PDF information.

So then all the terms sitting here the close term, they remain become closed or one can make it slightly more accurate in the sense in the description and close this term using velocity scalar PDF. So now this Reynolds stress component instead of closing from the RANS equation use the information of the Velocity PDF one can close this and similarly turbulence scalar flux one uses both the velocity scalar joint PDF and close it and the source term using scalar PDF.

So this will make things, now closed in the governing equations and the solution obviously as we said because of the dimensionality one has to adopt from some Monte-Carlo based technique.

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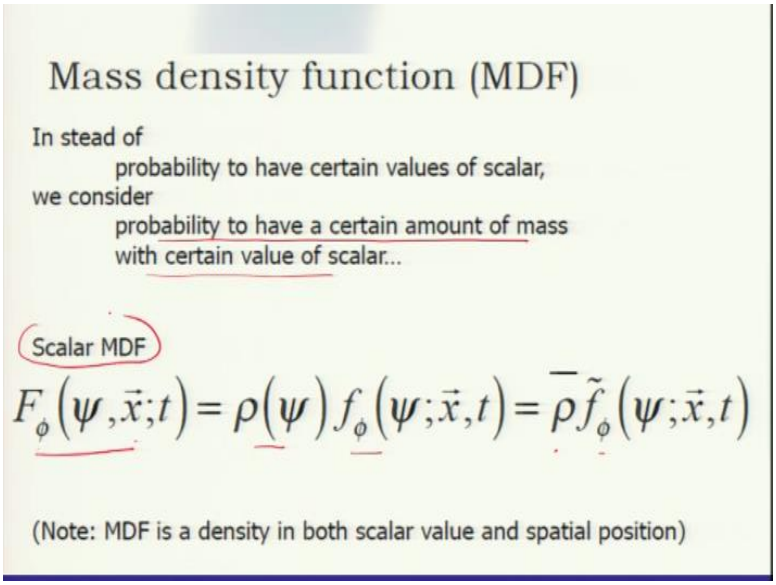

Now, we look at the mass density function, so instead of probably to have certain values of scalar, we say the probability to have a certain amount of mass with a certain value of scalar. So which will lead to this new definition, which is the scalar mass density function. So this is defined as

$$F_\phi(\psi,\vec{x};t) = \rho(\psi)f_\phi(\psi;\vec{x},t) = \bar{\rho}\,\widetilde{f_\phi}(\psi;\vec{x},t)$$

so this is our scalar mass density PDF or mass density function.

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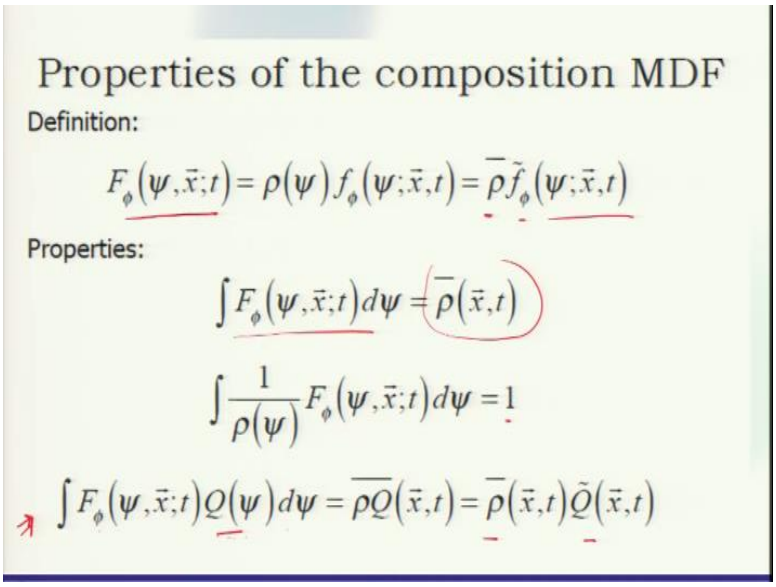

Now properties of this composition mass density function: so one can look at the different properties, like our mass density function is defined like this

$$F_\phi(\psi,\vec{x};t) = \rho(\psi)f_\phi(\psi;\vec{x},t) = \bar{\rho}\,\widetilde{f_\phi}(\psi;\vec{x},t)$$

So if we integrate this over dψ, this will get me the mean density and the normalization criteria also gives me 1. So one can write

$$\int F_\phi(\psi, \vec{x}; t) Q(\psi) d\psi = \overline{\rho Q}\ (\vec{x}, t) = \bar{\rho}\ (\vec{x}, t) \tilde{Q}\ (\vec{x}, t)$$

these decomposition would help to simplify some of the situation.

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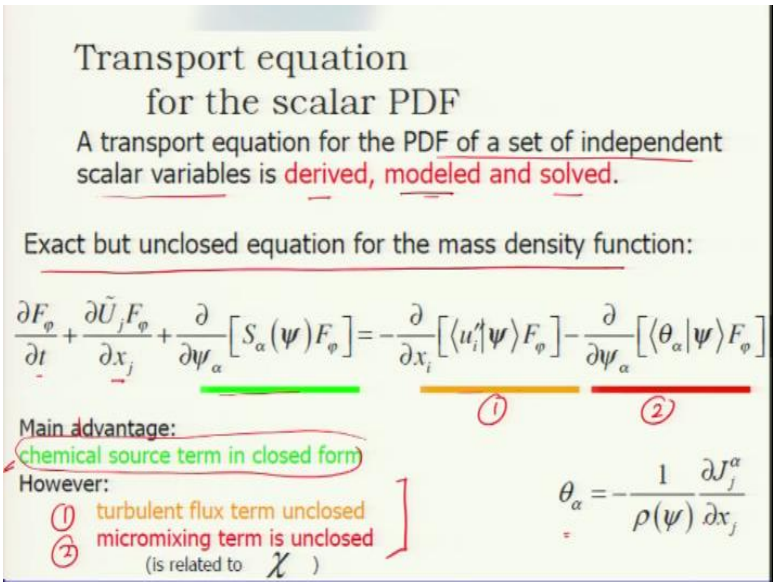

Now, we will look at our transport equation for the scalar PDF. So it is nothing but an equation PDF of a set of an independent scalar variable, which is derived, modeled and solved. When we say it is derived then there, would be some unclosed term. So because of this unclose term we can model this and then finally so we can see this unclosed equation of the mass density function, this will be written as

$$\frac{\partial F_\phi}{\partial t} + \frac{\partial \tilde{U}_j F_\phi}{\partial x_j} + \frac{\partial [S_\alpha(\psi) F_\phi]}{\partial \psi_\alpha} = -\frac{\partial \left[\langle u_i'|\psi\rangle F_\phi\right]}{\partial x_i} - \frac{\partial \left[\langle \theta_\alpha|\psi\rangle F_\phi\right]}{\partial \psi_\alpha}$$

This is 1 term, which is a term of chemical source term right-hand side. This is a turbulent flux and then this is the mixing term or the scalar fluxed. Here one of the advantages of this equation is that the chemical source term is closed from, this is one of the biggest advantages. Typically when you do the Favre averaging or density-weighted averaging our chemical source term in the mass transfer equation become unclosed.

So that gives or brings a lot of challenges to close that term and that is why we started discussing the simple reaction models or combustion models how to close the term. However, having this chemical source term in closed form, we still have other 2 terms on the right-hand side this term 1 and 2, this is the turbulent flux term and the micro-mixing term, they are unclosed.

So one needs some sort of enclosure for these 2 particular terms to be closed where theta alpha is the diffusion flux, which is defined as a regular ways.

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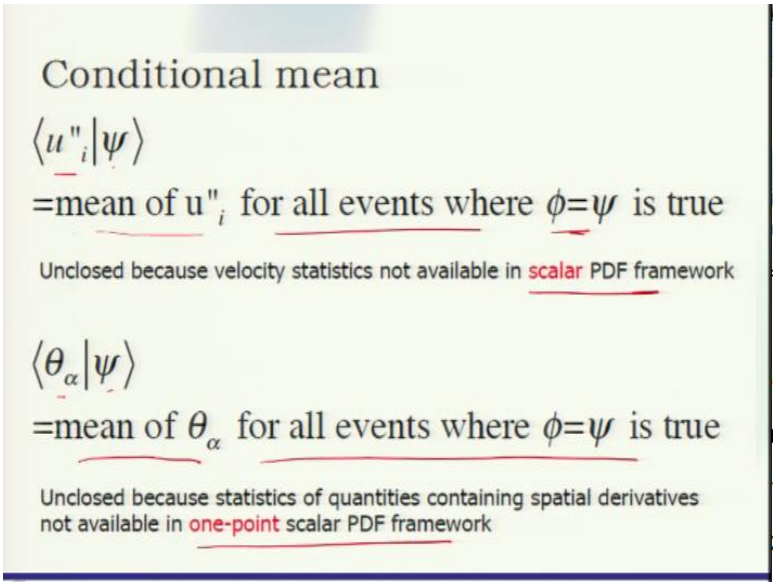

Now, once see this one know to look at this conditional mean: that means this term fluctuation of u which is conditioned on psi. It would be equated with the mean of u for all events where $\phi = \psi$ is true. That means it is a very simple way to close that particular term that contain that velocity fluctuation. So that allows that you consider the mean of fluctuations for all the events where you have $\phi = \psi$ which is true.

Now this term becomes unclosed because your velocity statistics are not available in the scalar PDF framework. So they are only the distribution of the available scalar quantities, so no information which is available for the velocity statistics. That is why we have to use some expression to close that term. Now the other term θ, α which is conditioned on ψ, which is the mean of θ, α for all events where θ ψ is true.

This is also unclosed because statistics of quantities, which are containing the special derivative or not available in 1 point scalar PDF framework. So since some information is not available, that requires closure of this term.

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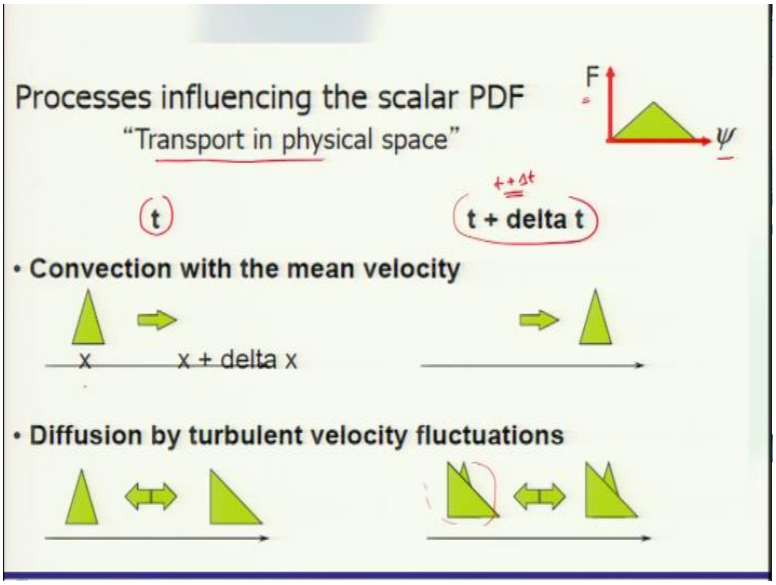

Now one can look at this particular process this is our function, this is in the variable space ψ. Now the process which influencing the scalar PDF now we can look at, this transport in physical space. So this is at a particular time t and this is at t + delta t. So what happens, this scalar PDF which is a known quantity would be again convicted by the mean velocity. So here if it is at x, x + delta x and this would be at this position.

Similarly the diffusion by turbulent velocity fluctuation, so this is the, at position x due to the diffusion of the fluctuation will be like this and similarly at t + delta t, this could be the shape and due to diffusion this could be like this. So that means 1 and there is an effect of the combustion convection. Secondly, there is an effect of these things.

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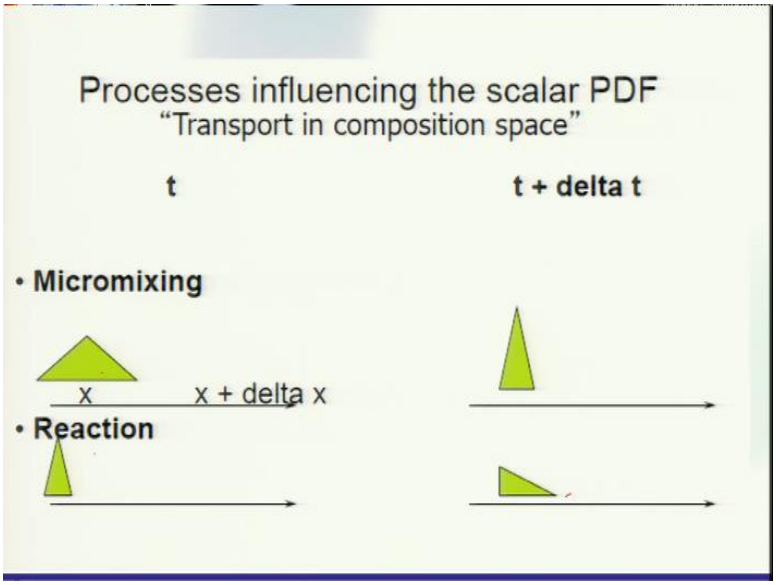

Now, then similarly micro-mixing term, so here is position x then t + delta t, because of micro-mixing, so it takes in different shape. Similarly, due to reaction at next time level, this becomes like this. So reaction will essentially lead to the consumption or destruction of some consumption or production of some of the species and that will be like that.

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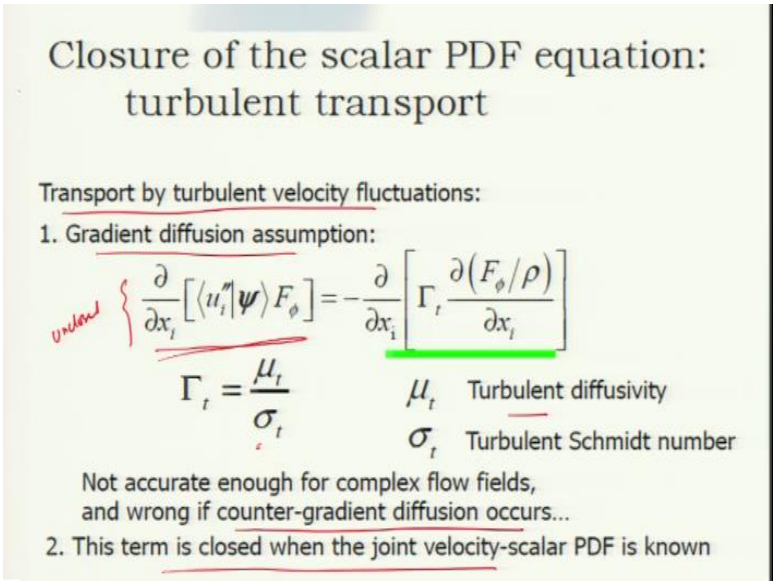

Now we can look at the closed form of this scalar PDF equation, so, we are looking at the terms which are on the right-hand side. These are the terms that we talked about this right-hand side term and the, is a one-term which is transferred by the turbulent velocity fluctuation, so we use the gradient diffusion assumption and we write this term which is unclosed, this is a unclose term.

It is like

$$\frac{\partial}{\partial x_i}\left[< u_i''|\psi > F_\phi\right] = -\frac{\partial}{\partial x_i}\left[\Gamma_t \frac{\partial\left(\frac{F_\phi}{\rho}\right)}{\partial x_i}\right]$$

Where

$$\Gamma_t = \frac{\mu_t}{\sigma_t}$$

Now, this is an simplest assumption or very common assumption one can use this gradient diffusion assumption bar for some flows this may fail. Now accurate enough for complex flow field, but this will fill if there is a counter gradient diffusion occurs.

So this is most of the wide range of cases this works nicely but in certain cases, this fails where the counter gradient takes place. Now, this term is closed when we take joint velocities scalar PDF, but since the velocity statistics is not available from the scalar PDF information, that is why we have to close it and the simple way to close it is this. Now the second term on the right-hand side, which requires closer of this term.

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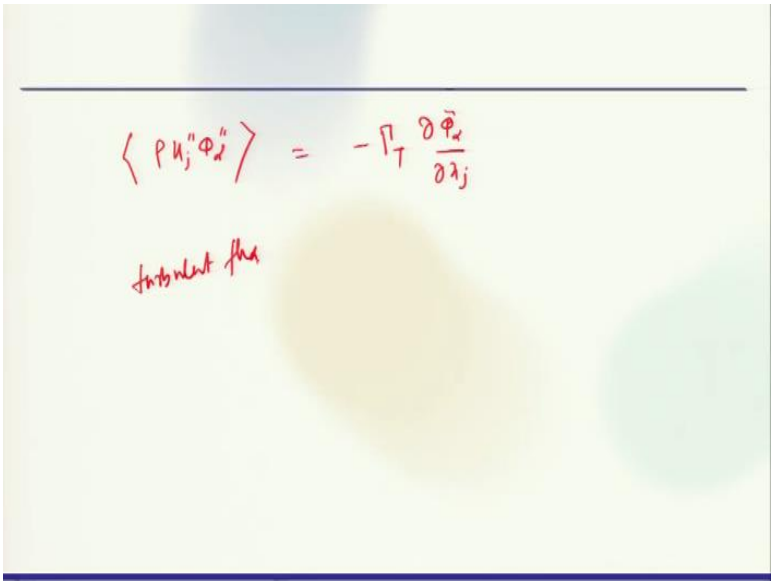

The fluctuating of the system also uses the gradient assumption we use this is the turbulent flux term. So we close it by the simple mean.

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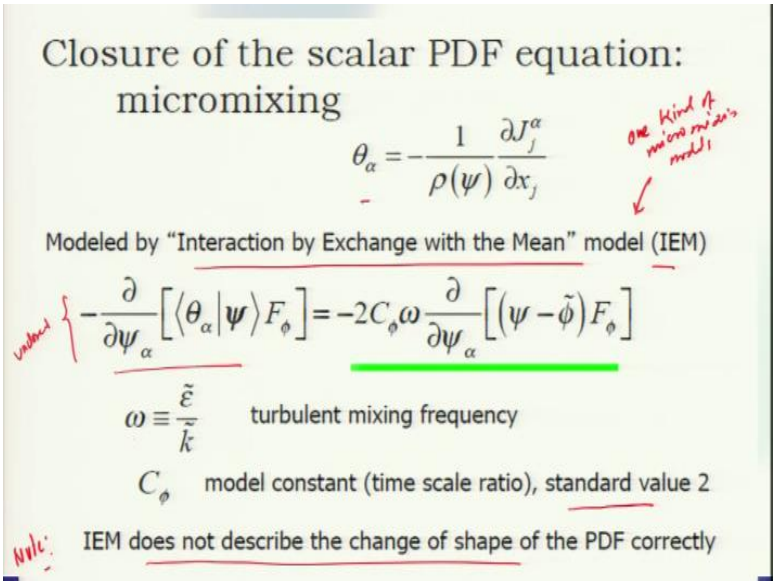

Now the term which is there another term is the

$$\theta_\alpha = -\frac{1}{\rho(\psi)} \frac{\partial J_j^\alpha}{\partial x_j}$$

How do we do that? So we use some micro-mixing model, so this is an interaction by exchange and mean this is one kind of micro-mixing models and more details can be found in some of the review literature and also there is a book by Rodney Fox where all these micro-mixing terms are discussing details.

So this is called introduction by exchange with the mean, IEM model, which is a very common and well-known model. Now, when we look at this gradient term, which remains unclosed in the PDF transport equation, we close it by $2C_\phi\omega$ and the gradient of delta alpha with respect to this where ω is the turbulent mixing frequency and C_ϕ is the model constant, which is a time scale ratio.

The typical value, which is often used, is 2. So for a wide range of flows, this works fine, but obviously having said that it also needs some tuning when there is a change in time scale. That means if some flows which are kinetically controlled that time one has to treat this parameter a bit to take into account that thing that the kinetically controlled situation. But another point one has to note here is that this IEM model does not describe the change of shape of the PDF correctly, but this is simple enough to essentially close this mixing term.

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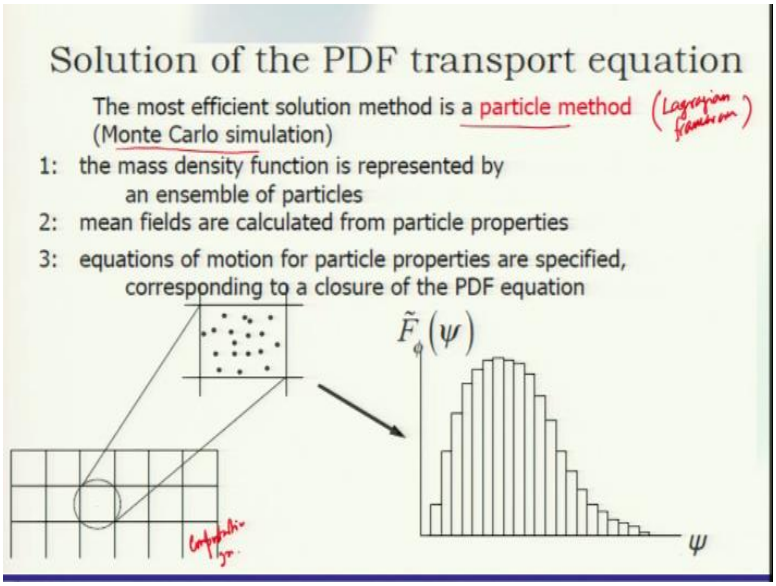

Now, we can look at the solution procedure of the PDF transport equation, and as we have already discussed the most efficient method would be particle-based method the Monte Carlo

solution. That means you need a Lagrangian framework to solve it because the dimensionality of the transport equation of the probability density function transport equation is so high one cannot solve in a regular methods like your numerical methods like finite difference or finite volume kind of approach.

So it requires some special treatment and the special treatment is like that it is solved in a particle-based method or in the Lagrangian framework, which is often known as Monte Carlo simulations and this is proposed by Steven Pope. So the mass density function is represented by an end symbol particle that means if you look at this is your computational grid so for each cell there will be a large number of particles.

And these are not massless particles and they will represent the mean properties of this particular cell. And if you look at the distribution in the composition face, this is the mass density function distribution. So mean fields are calculated from the particle properties, obviously and then when the equation of motion of particle properties are satisfied it corresponding to closer of the PDF equation.

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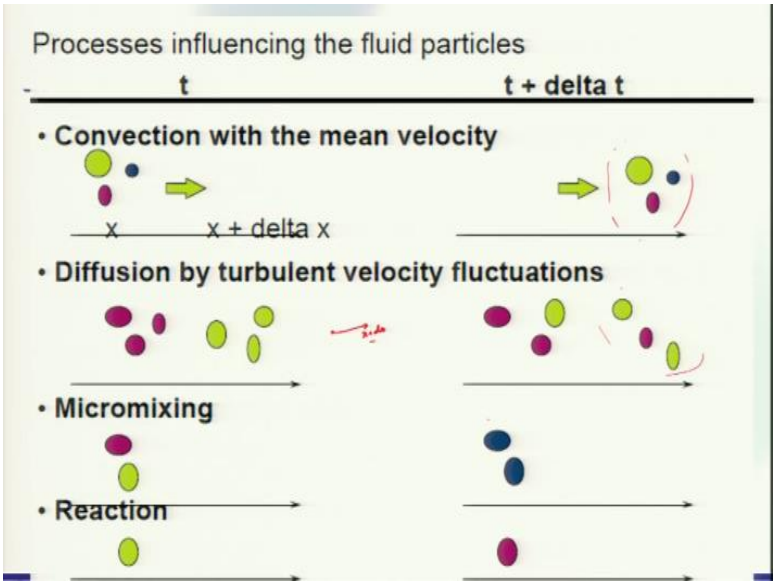

Now, the process which influences the fluid particles, there would be convection like convection due to mean velocity. So let us see if the particles are here at this position at the next time step because of this convection effect or the convection effect of the mean velocity particles reach. So that is like you have some particles like your, you can think about your food particles which are always convicted downstream due to convection.

Secondly, there could be diffusion by turbulent velocity fluctuation, that means let us say particles are here in the next special coordinate system or if they are here and then goes to x + delta x because of this diffusion, they come here similarly the particle by the time next time step if there come here and then the diffusion also impact then there could be mixing, so because of the mixing you can see how they behave.

And then finally reaction will allow taking into consideration of the scalars the reactive scalars which are either getting produced or consumed during this process.

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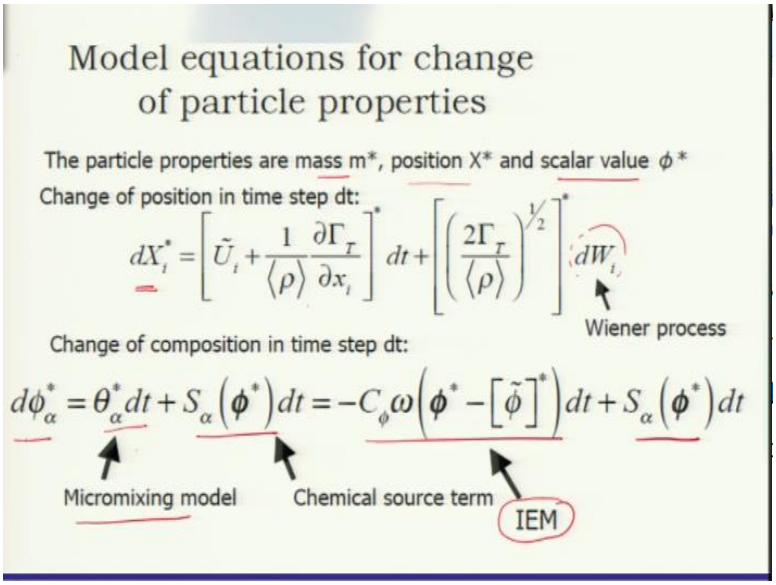

Now, how do we model these particle properties or the change of particle properties? because we have already said that each compression cell will have some number of natural particles and these particles do have some mass. These are not massless particles and the particles collectively in a particular cell will determine the macroscopic properties of that particular computation cell.

So these are very essential properties. So as you said the particles are having some Mass they also at a position X and the scalar which is carried by this particle are 5-star. Now change of position in time step dt so from one position, so there will be delta exchange for a particular particle. So this is due to the mean flow field and the gradient plus the other part and the Wiener process.

So this is a random process which will allow the particles to move stochastically. So this wiener process is known as in stochastic process. We allow these particles to move randomly within

that particular cell, but with the combined effect we can see what would be the displacement of these particles over a time stable duty. Now similarly that we change of composition in time step of dt and that also we can see if this is $d\phi_\alpha^*$.

This is the phi alpha dt, that is coming from the micro-mixing model and this is due to the source term of the chemical source term which allows the particle to get me there are 2 components 1 is mixing 1 is a reaction and the reactions are going to say how much is consumed or produced and something like that. So the mixing model is closed like this using the IEM model which we have already discussed.

And then this is the source term chemical source term, which will also tell you how much there will be change in composition because of this time step check.

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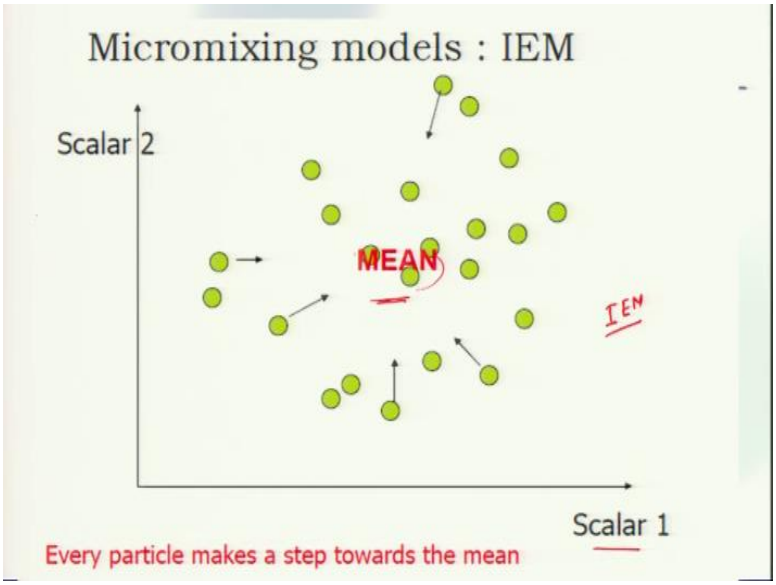

Now, we can see the micro machine model behavior how that behaves. So this is what you can think about in this direction, there is one scalar which is in this direction, there is another scalar and this is all the particles and let us say the mean properties would be somewhere else. When the tendency of this each particle is to go towards the mean and that is why we call it IEM interchange by exchange and mean.

So this is how the in mixing phenomena or in the context of the mixing phenomena you can think about this is going to be the particle behavior. So they are random or their position is going to be determined randomly through this wiener process and all these things and also the

effect of mean and the other fluctuations but still in the mixing level, they have a tendency to go towards the mean, so this is how IEM model actually captures this particular phenomenon.

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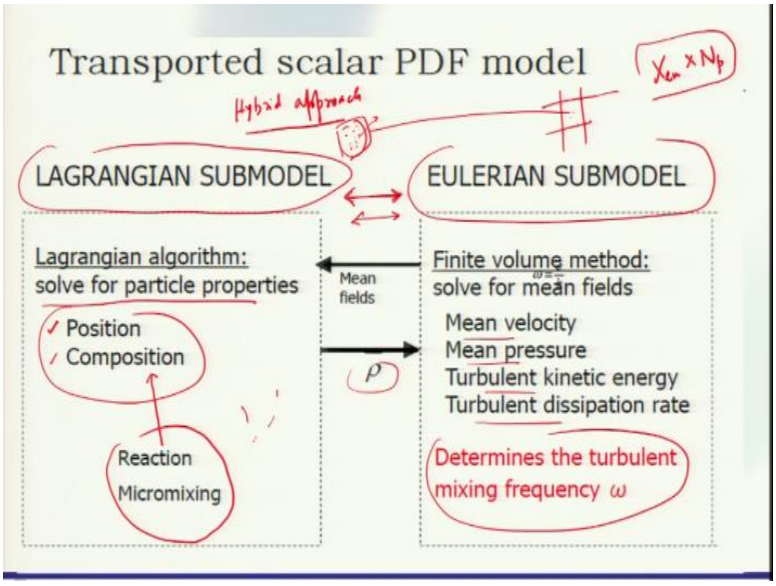

So if we, somehow put up together the process of this transport scalar PDF then we can see this is a sort of a hybrid approach that means you have both already Eulerian sub-models and you have Lagrangian sub-models also. The reason is your PDF distribution function of the PDF transport equation cannot be solved completely in the Eulerian framework and the preferred or most preferred or most efficient solution algorithm is the Monte Carlo algorithm, which is the particle-based Lagrangian algorithm.

So, which essentially makes this particular approach to be a hybrid approach. So what do you have in your eulerian sub model? If you look at it, so you have some finite volume method to solve for mean fields, which will solve mean velocity, mean pressure, turbulent kinetic energy, dissipation rate and you can determine the turbulent frequency from here, which is essentially epsilon by K.

Now, this is solved in your Eulerian framework, and this particular set of information you send it back to the lagrangian framework or lagrangian sub-model, but the lagrangian some model you look at individual particles. What you look at, you look at their position so due to this randomness and the top of that the effect combined effect of the mean fields and the randomness how their position changes and also the change in the composition.

These are the 2 things that are very important and then this change of composition is impacted by reaction and micro-mixing. So these are also important sub-model in the Lagrangian framework. So once we do that, then the particles randomly move from this place to that place and so but still there would be a collection of particles that sit or stay inside the one particular cell or computation cell.

But another thing here to note there once a number of particles which stay inside the competition cell already on cell, so that is where you find out the macroscopic properties like density, which is again sent back here and this is where and also one has to make sure that the global mass conservation is not violated, that means any eulerian cell which will have the corresponding particle cell particles there.

So the mass conservation this is the sum of the total particle mass should be the same with this. This is one thing there is a checking which is constantly done to happen proper handshaking between these 2 frameworks and then also one has to account for let us say you start by assuming, n number of particles in each computational or already and greed then due to these fluctuation randomness of the motion position the particle may cross the cell boundary.

So if that happens you have to immediately account for that information. So these particles move to the other cell where there would be n plus 1 number of particles but then through the mass conservation or global mass conservation you redistribute the mass amongst those particles into a number of particles. Similarly when there is a loss of particle from a particular cell then again.

You look at the global mass conservation from there redistribute the mass to the n number of particles. So these are the things one has to take into account. Well, there is an information transfer between these 2 sub-models and the solution process or progress in this fashion. But when you have this hybrid kind of model still it requires a lot of memory. The reason is the following.

You have already a cell which could be of the order of a few thousand million cells depending on the problem. But now each particular Eulerian cell will have n number of particles then your number of particles that we are dealing with that X number of Eulerian * n particles.

So that many particles you are to in totality dealing with so that is the still memory requirement are high.

Then, since the solution is going back and forth between these 2 sub-models already in a Lagrangian framework it is slow but when you pay the price in the sense, it is quite accurate and gives you because this captures the randomness of the motion.

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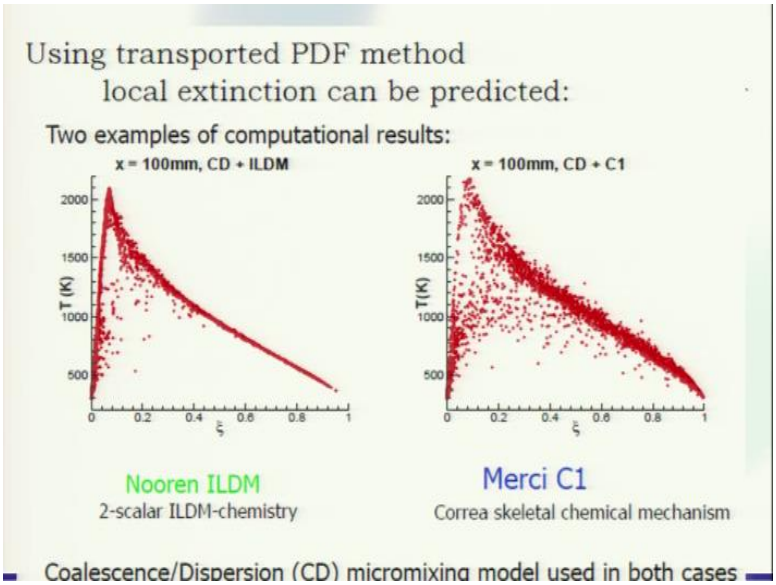

This is an example which will be picked up from a transported PDF calculation for the local extension that was predicted, so this is using natural gas.

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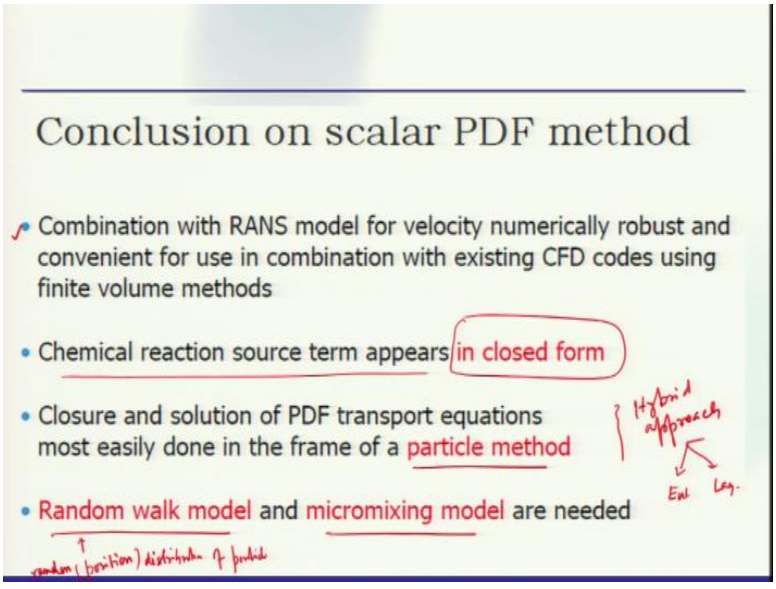

So if we, I mean put the points together for this scalar PDF discussion. So the combination with the RANS model for velocity numerically robust and convenient for use in combination with

existing CFD code, like the finite volume method. So this is how we combine with the RANS framework that is one of the advantages. Then the second advantage is that the chemical source term appears in closed form.

This is very important because this is one of the terms which is which creates a lot of problem along with challenges to close it in a governing equation. After all, that is quite steep and make the system of the equation to be quite steep enough for a solution. Then closure and solution of PDF transport equation and mostly done in the framework of particle method or rather I would say it is a hybrid approach which is adopted.

So this has both Eulerian and Lagrangian. So the combinations of these 2 give you the best solution method and then we use random walk model this is for position or random position or rather distribution of particles. So this particular model will allow to estimate the random distribution of the particles and micro-mixing model to close the unclose term in the mixing phenomena.

So this is what one can see how we get the solution of a scalar PDF transport equation. So we will stop here and continue this discussion for the velocity scalar PDF and we will look at how one can obtain the solution and what are the issues and how to close those particle positions and they are mixing in the next lecture. Thank you.