Turbulent Combustion: Theory and Modelling
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Lecture - 48
Turbulence- Chemistry Interaction (contd…)

Okay, welcome back. So we are in the middle of the discussion of this PDF transport, a PDF-based approach and we have now looked at the solution procedure starting from the governing equations the scalar PDF approach. Now, we will continue the discussion for the velocities scalar approach.

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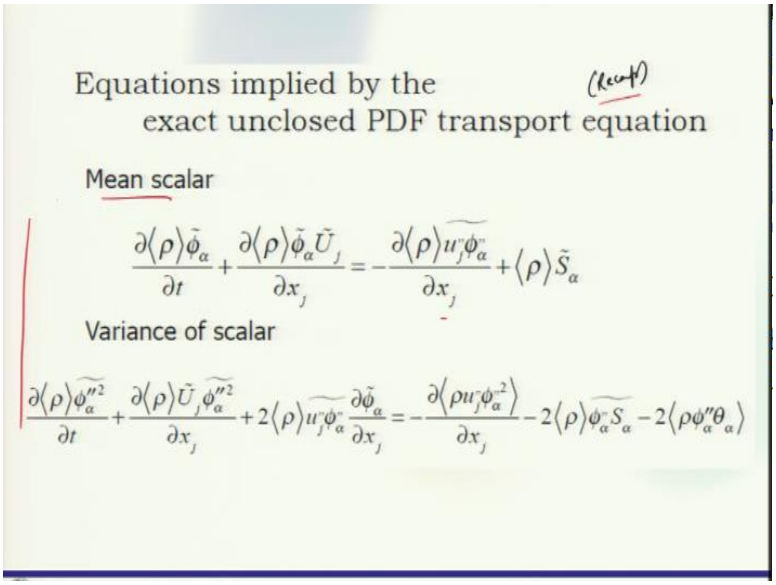

Now to recap the equation system, so these are mean scalar and in the density-weighted system, so the mean scalar is written, this one, this is the flux and this is the variances of the scalar. It is a quite standard equation so any textbook, any material that can look at you will find the set of equation. So I am going into term by term of this particular equation as such because they are the standard set of the equation that is available in any standard textbook.

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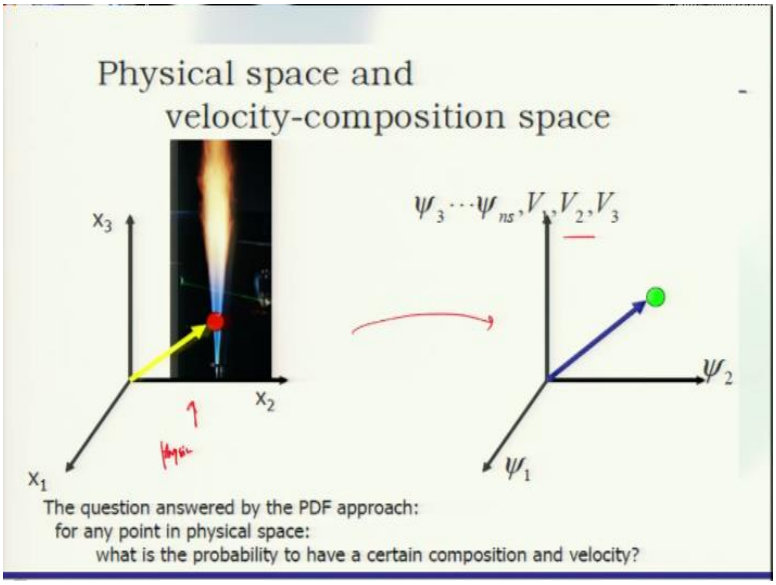

What is important? We will move to the discussion of the now velocity composition space, so this is our physical space, where the flame is there. It is an unconfined flame and when you come to this physical space to compute velocity composition space you have all scalar composition along with the velocity components. So they will form this sample space where we try to find out the probability to have certain composition and velocity of the information.

So this is 1 point statistical calculation or analysis where we try to see them from the probabilistic approximation or distribution, we try to see the that information availability.

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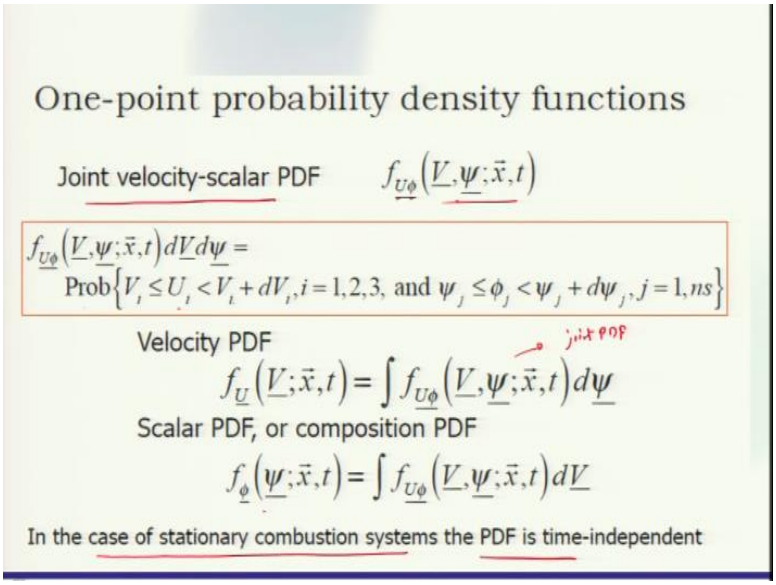

So one point probability density function: this is how we define the joint velocities scalar PDF where you have the velocity component in the scalar, so this is how you define the PDF function. Now if the PDF function if you look at that the probability of finding this velocity

component between these limits and the scalar composition between the limit. Now we can get back the pure velocity PDF if we integrate this over the sample space will get back the this is joint PDF from which we can get back the velocity PDF and this is the joint PDF.

If we integrate over scale velocity space we can get the scalar or composition PDF and as we mentioned earlier that case of stationary combustion system the PDF is time independent.

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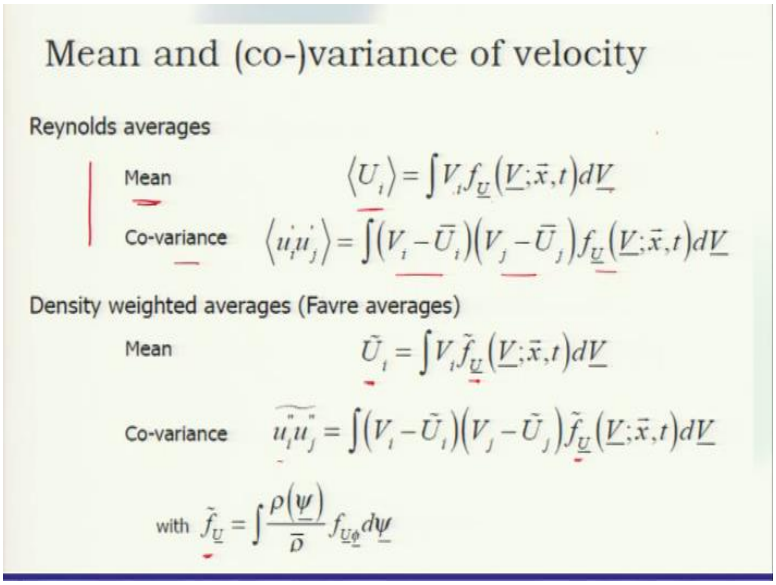

Now once we look at this joint PDF, we can see this different component after Reynolds averaging. So there would be mean there could be covariance and all this. So the mean quantity we can find out this is the mean which is within the bracket like this. This is an integration of the velocity of velocity PDF over the velocity space. So this is essential as we have seen earlier the N = 1 this is n^{th} moment but 1.

Covariance where n is 2 so that is the difference of 2 velocity components and the integration of this PDF function over the velocity space. So that is how you get the mean and covariance and these are the terms which would be required to close some of this unclosed term arise in the equation. Now once you do Favre average, this is the Favre average mean, so then we will take the fabric average PDF function.

Similarly for covariance would take the Favre average PDF function where the Favre average PDF function is defined as

$$\tilde{f}_{\underline{U}} = \int \frac{\rho(\underline{\psi})}{\bar{\rho}} \tilde{f}_{\underline{U}\,\underline{\phi}} d\underline{\psi}$$

So this is how you get to this thing.

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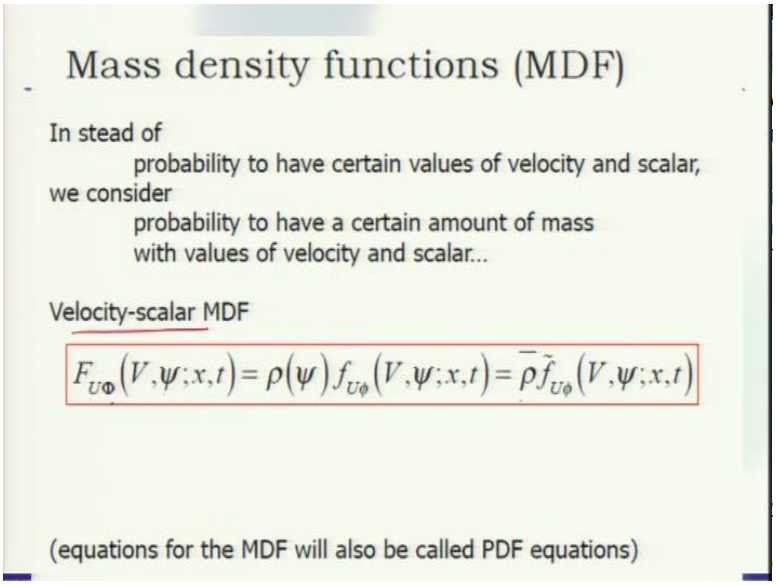

Now we can also define the mass density function where instead of having a probability to have certain values of velocity and scalar, we now consider that probability to have a certain mass with the values. So now we will is it is scalar must density function which will be defined $F_{U\phi}$ which is on velocity and scalar $\bar{\rho}$ and so the equation of this MDF would be also a similar transport equation for the PDF.

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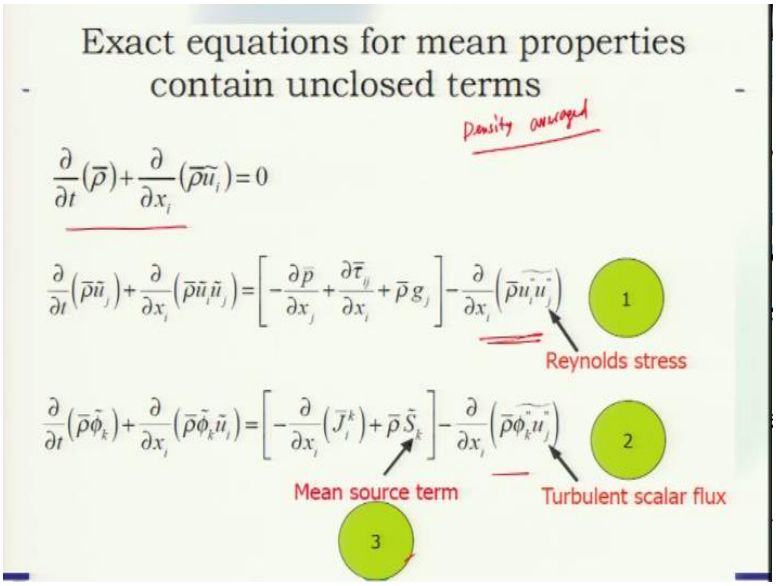

Now when you come to the exact equation of these mean properties, which contains the unclose terms, this is again density averaged quantities so this is the term Reynolds stress term which

is unclosed, turbulence scalar works is enclosed and source term and will now close them using our concept of this velocity scalar PDF.

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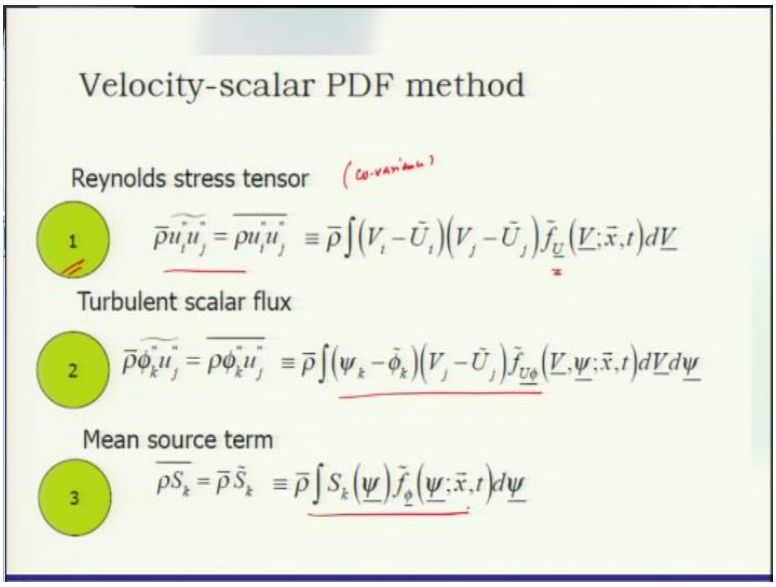

So the term which you get the Reynolds stress term now instead of using any RANS equation or k epsilon equation now, we close them using the information of our velocity PDF. So that means when you have that PDF distribution function using that this is our, you think about this is the covariance that we have already discussed. Then the turbulence scalar flux we use the velocity scalar PDF to close this turbulence scalar flux.

So we do not use any information or gradient assumption or something like that to close that term and finally the source term as usual we will close using the scalar PDF.

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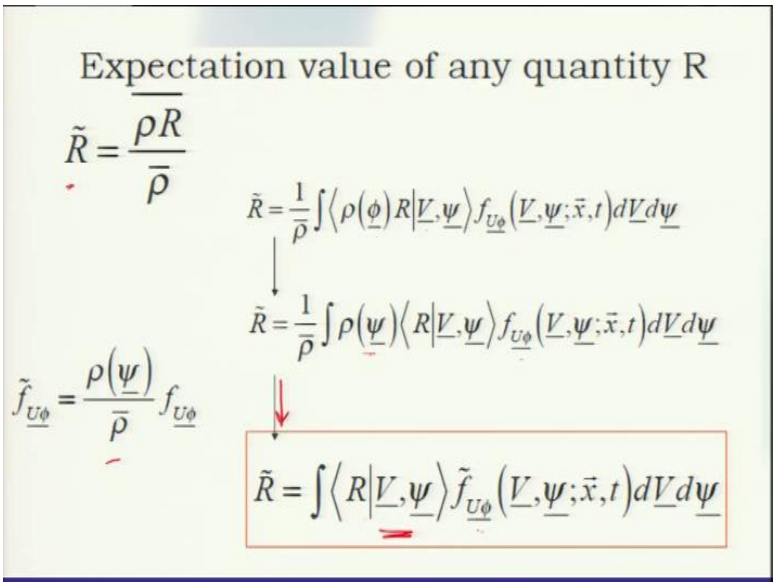

Now if you look at the expectation value of any quantity R so this is density otherwise R, the expectation value would be

$$\tilde{R} = \frac{1}{\bar{\rho}} \int \langle \rho(\underline{\phi}) R | \underline{V}, \underline{\psi} \rangle \, f_{\underline{U\phi}} \left(\underline{V}, \underline{\psi}; \vec{x}, t \right) d\underline{V} d\underline{\psi}$$

Now if we rewrite that, this would be

$$\tilde{R} = \frac{1}{\bar{\rho}} \int \rho(\underline{\psi}) \langle R | \underline{V}, \underline{\psi} \rangle \, f_{\underline{U\phi}} \left(\underline{V}, \underline{\psi}; \vec{x}, t \right) d\underline{V} d\underline{\psi}$$

$$\tilde{R} = \int \langle R | \underline{V}, \underline{\psi} \rangle \, \tilde{f}_{\underline{U\phi}} \left(\underline{V}, \underline{\psi}; \vec{x}, t \right) d\underline{V} d\underline{\psi}$$

This is my density or Favre mass density function and so this is where the density weighting helps to find out that expectation value at conditions at V and ψ. So this will give you an example. Now the reason is that why we want to see how one can estimate that expected value then we can use that.

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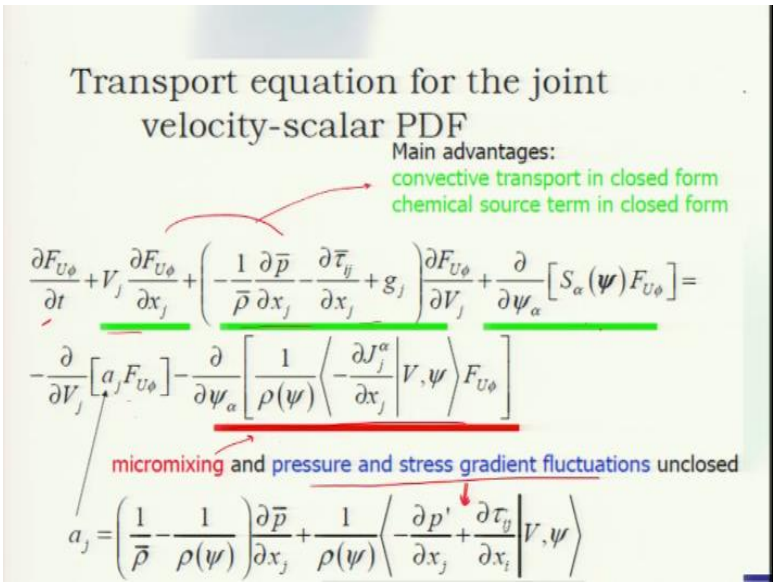

Now, this is a transport equation for the joint velocity scalar PDF. Here this is the term, this is convection, this is another term, this is source term. This is the term on the right-hand side. Now if you look at it the term here on the left-hand side the chemical source term that is in closed form. So that is one of the advantages of the joint PDF equation or the PDF transport equation because chemical Source term which actually in cars lot of stiffness in the system so that is unclosed form.

And then the convective transport is also in the close form so these 2 terms are also in the closed-form. So these term on the right-hand side is the acceleration term, which is also basically these particular term is the micromixing term and here there is a fluctuation of pressure and stress gradient, which is also unclosed. So this is unclosed, this guy is unclosed. So there are 2 terms but this is in the this is a gradient of pressure.

So this remains closed but the component of that which is a fluctuation of pressure and stress gradient, remain unclosed in the system. So, one has to handle that properly to close these terms. Now if you immediately try to see the difference between your scalar PDF and the velocity scalar PDF the governing equation starting from the governing equation, it becomes little bit involved or more rigorous in that sense. Because, as long as you had only scalar PDF, you never had this term, which is arising on the right-hand side.

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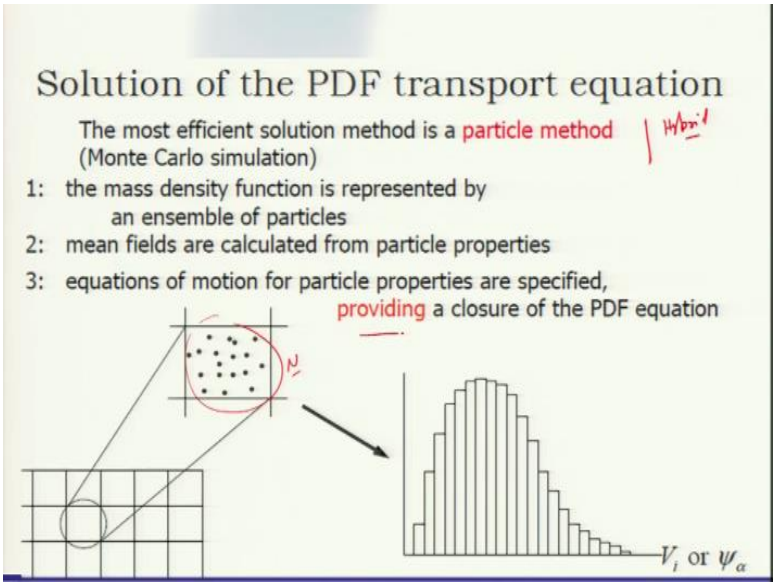

So a solution procedure would be in a similar fashion, so you need a hybrid approach that means you will solve some of the mean quantities in the Eulerian framework then each compression framework which has some in number of particles. These particles are going to have some mass, they are not mass-less particles and they will also expose to the reaction mixing and turbulent fluctuation.

So they will change their position randomly, they will be affected due to mixing and reaction-diffusion through all sort of things would happen to this particle field and finally, there would be a conservation of the global mass for each of these computers on cell and the information

would be passed back to the Eulerian framework. So there is handshaking which will be required between your 2 frameworks that is one is the Eulerian, the other one is the Lagrangian.

Then this information will be obtained from the particle properties, they will provide the closer form of the unclose term in the PDF equation.

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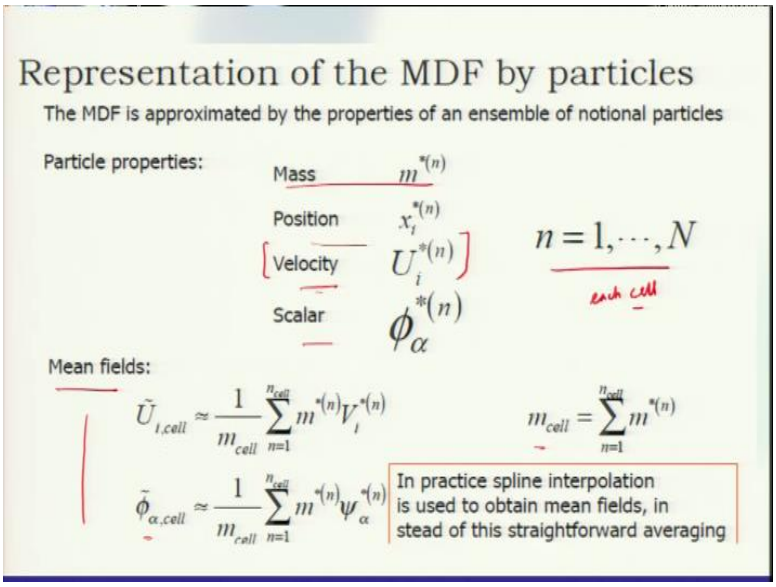

Now when you look at the mass density function by particles for velocity scalar PDF, it is are you have some notional particles, n number of notional of particles, there would be there in each cell. So they are having a certain mass, they will be at a position. There will be some velocity and there would be some scalar now previously when we looked at the scalar PDF this is the 1 component or 1 term which was not required there.

Because it is only the scalar PDF that we are discussing and any velocity statistics were not available or the information related to velocity statistics was not available from the scalar PDF. But here we have a joint velocity PDF velocity and scalar PDF. So the statistics of the velocity field are available. So that is why these for the particle will also become important then when you look at the mean fields, we total number of parcel the mean velocity component means scalar component and the mass.

So these are the important parameter that one has to satisfy to keep it or make the cognizance between the Eulerian framework and the particle framework. So there is a simple interpolation, which is used for averaging and all this one can use some more complicated interpolation.

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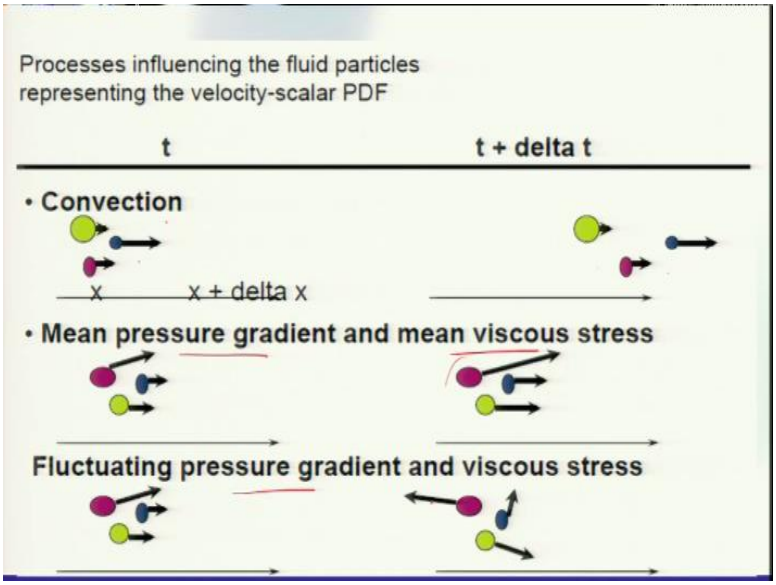

Now we will quickly look at how the things would, particles would react to different kinds of phenomena. So there will be convection, so the particle will move to change its position, time. There is mean pressure gradient and mean viscous stresses for that, they will expose to also different stress components and there is a fluctuating pressure gradient in this viscous stress. So that will allow the particle to show a different kind of behavior. Then obviously there will be mixing and then reaction.

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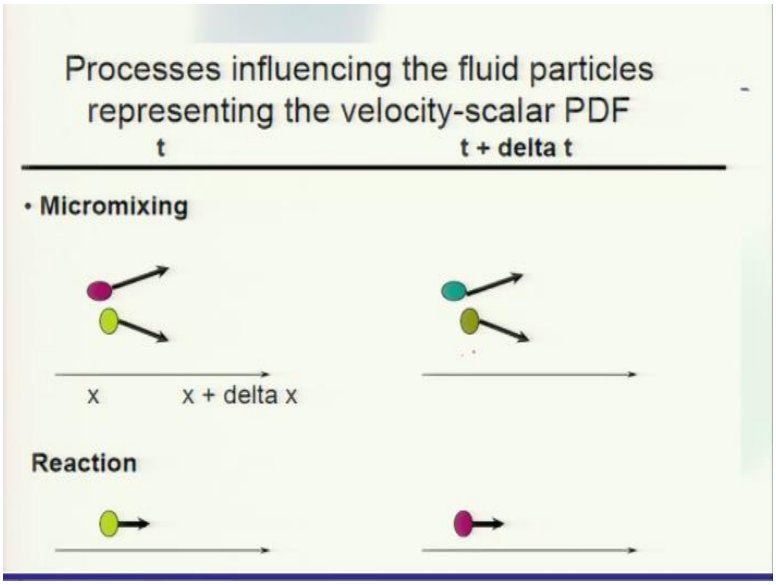

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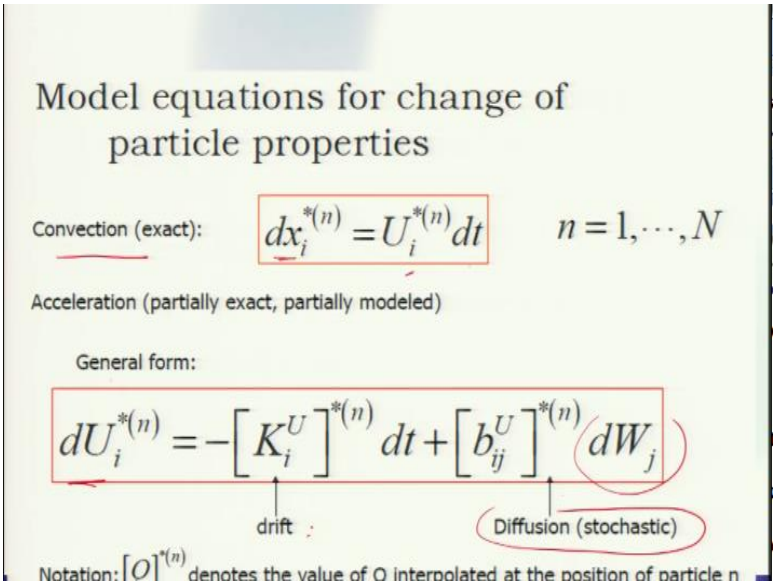

So they will sort of react to all these different phenomena which will be occurring in the particle framework. Now the model equation for change of particle properties, first thing there would be a convection of the particles. So then the displacement can be estimated for an individual particle like the $U_i^* dt$. Then we can have the acceleration part which is partially exact and partially modeled.

The general form of that change of the velocity would be because of the drift and diffusion, so this is the wiener process. So this process is completely stochastic, this drift can be estimated also, different stochastic model.

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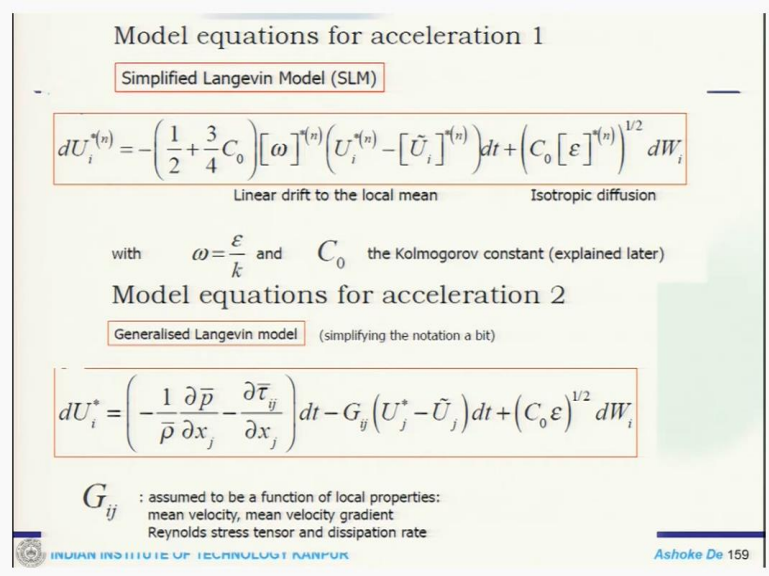

Now there are model equations which are often used for acceleration, now one is simplified Langevin model, which uses this dU_i^* is like

$$dU_i^{*(n)} = -\left(\frac{1}{2} + \frac{3}{4}C_o\right)[\omega]^{*(n)}\left(U_i^{*(n)} - [\tilde{U}_i]^{*(n)}\right)dt + (C_o[\varepsilon]^{*(n)})^{1/2}dW_i$$

ω is nothing but the turbulent frequency and there is a difference of the instantaneous and mean velocity and then there is an isotropic diffusion dW, so this drift here, which is calculated this is a linear drift to the local mean.

So that means that is why this is known as the simplified Langevin model and the C_0 here, which is the Kolmogorov constant, which we will explain a little later and but then there is another model which is a generalized Langevin model how it calculates this drift that it this is a diffusion which is a Wiener process, then it has a pressure gradient and stochastic gradient and then there is a process.

So this function G is local properties mean velocity, velocity gradient, and station dissipation rate and how that look like?

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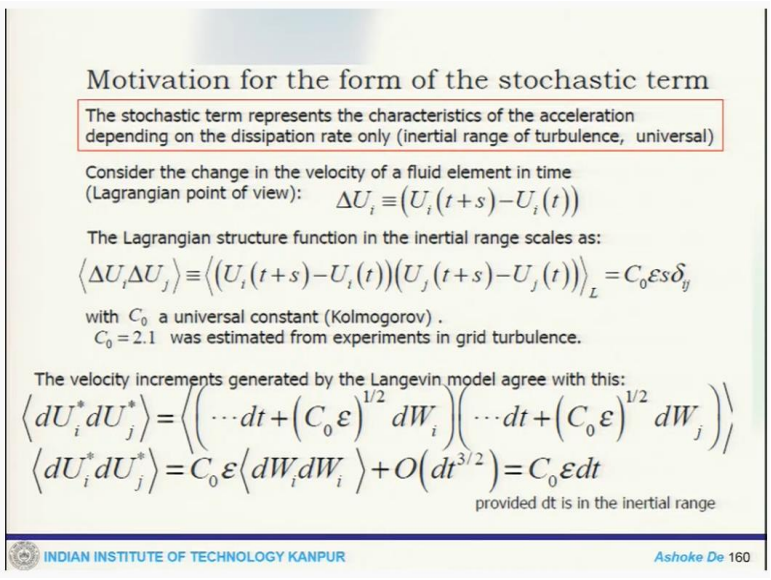

Now the idea or ideology behind that is that the stochastic term represents the characteristics of the acceleration depending on the dissipation rate only. So that means it is in the inertial range of turbulence and universal, so now if we change of velocity from the fluid element.

This is from Lagrangian point of view this should be

$$\Delta U_i \equiv (U_i(t+s) - U_i(t))$$

Now the Lagrangian function of the inertial scales would be

$$\langle \Delta U_i \Delta U_j \rangle \equiv \langle \big(U_t(t+s) - U_t(t)\big)\Big(U_j(t+s) - U_j(t)\Big)\rangle_L = C_o \varepsilon s \delta_{ij}$$

So this is a universal constant which will be 2.1. Now similarly the velocity increase increment due to the Lagrangian model nicely correlates with this concept.

And this is where you get this term and the other part and this particular part is correlated like this and this is the so this is in the sort of in your inertial range. So, that this is coming from actually stochastic physics, where you try to see the consistency between your other phenomenons.

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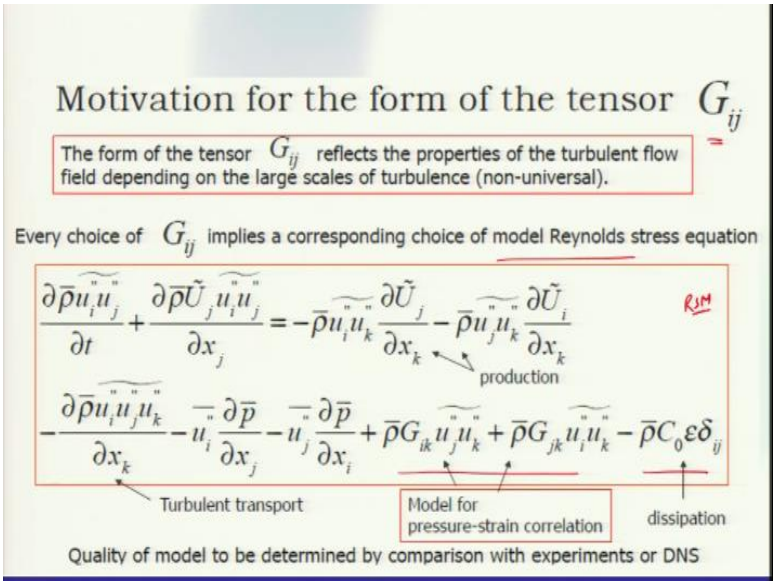

Now G_{ij} is another important term sitting there which will reflect the properties of the turbulent field depending on the large scale of turbulence. So that means if you go back here, this will depend on the large scale and which are non-universal. So now if you look at the choice it is a corresponding choice of the model the Reynolds stress equation where the stress individual stress term is looking like this.

These are production terms, these are the term and this is the term which comes from the pressure-strain correlation and this is the dissipation. So one can look at this is Reynolds stress

model in RANS framework where they can look at how these terms and then make a choice which will make it corresponds with that.

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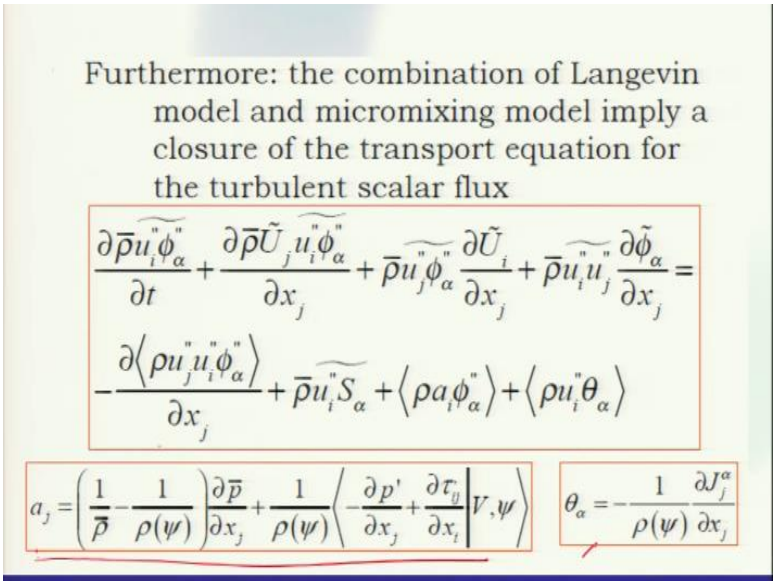

Now further, there will be combination of Langevin model and macro mixing model. So that will close down the transport equation for the scalar flux. Now if you look at the scalar flux, this is how you get and this is the term which will appear in the closure of that and this is the theta alpha.

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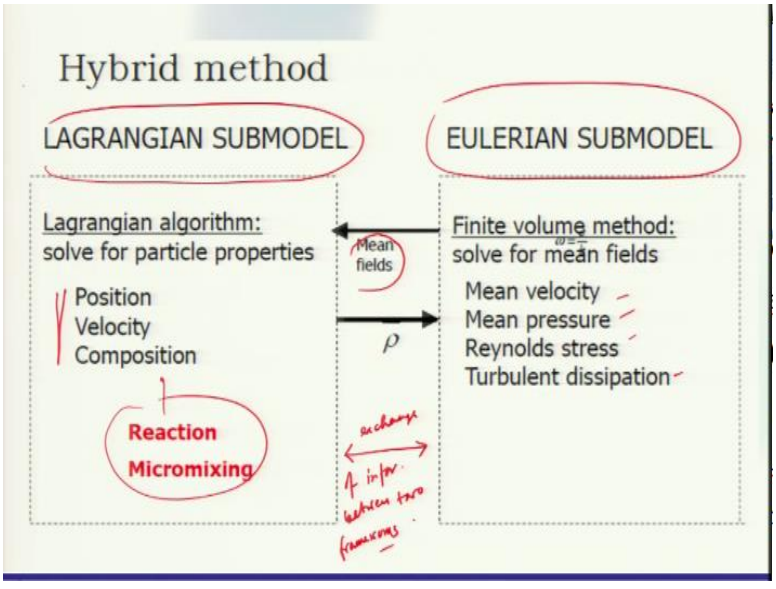

So that is how you close this term and then you go to the solution approach, which is again in the hybrid framework. That means you have an Eulerian sub-model where you solve mean flow fields in the Eulerian framework and then you go to the Lagrangian sub-model while you solve the particles. So here you solve for mean, velocity, pressure, stress, turbulent dissipation

and this mean information you pass to the Lagrangian where you solve for the position, velocity, composition with the impact of reaction and micromixing.

So by doing that what you do that when you look at the global parameters like mass conservations, density and the particles when it is crossing out of the boundary or it gets into a different bound cell. So all these they are doing that so there is a constant exchange of information between 2 frameworks so that is what it does.

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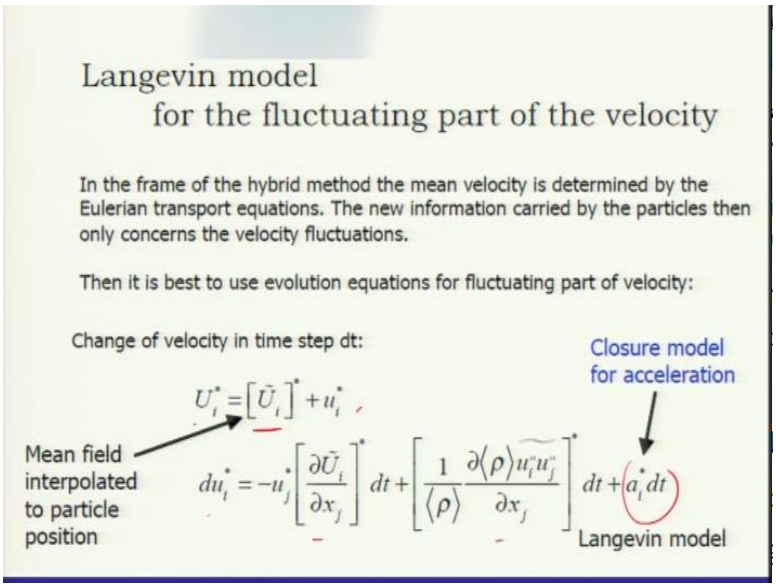

Now the Langevin model if you look at the fluctuating part of the velocity where the mean velocity is determined in the Eulerian framework, but the particle framework when you look at their the change of velocity of the particles is his duty to do to mean-field and then these small components where the change is approximated like the velocity gradient flux and the acceleration term which is closed by the Langevin model or generalized Langevin model like that, so that is what you get this positions and the velocity of the particles.

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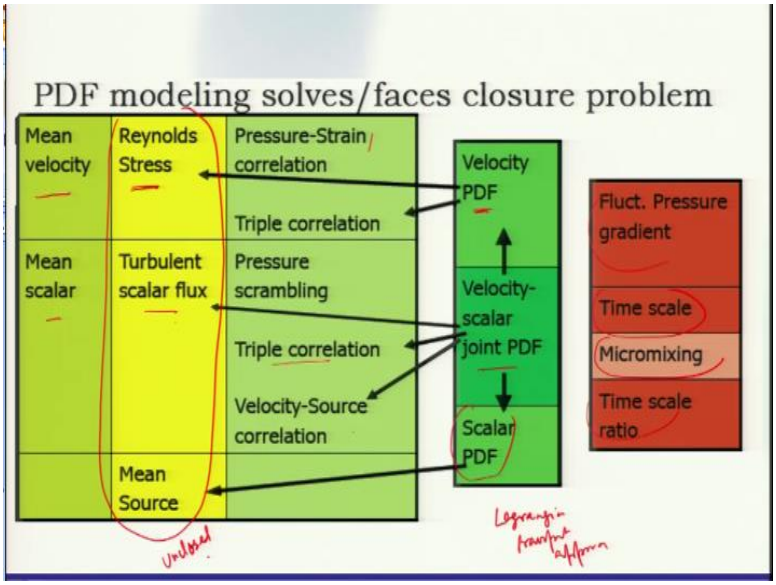

So if you put up the whole set of discussion on this scalar PDF or transported PDF in one particular these things then you can get this is our velocity scalar PDF, this is both velocity joint scalar PDF and this is scalar PDF. So from joints scalar PDF, you can still achieve your velocity PDF and also scalar PDF and the other term you have time scale your micro-mixing, time scale ratio pressure fluctuation gradient.

So when you look at the velocity PDF using the velocities PDF, you close the Reynolds stress term, and also you have pressure strain correlation and triple correlation that is closed using this velocity PDF and this is where mean velocity and means scalar you get from the Eulerian framework now, using your joints scalar PDF turbulent scalar flux and velocity source correlation and the triple correlation.

So these are the term which you close using the information of the joint velocity scalar PDF and only using the scalar PDF you close the mean source term. So that will give you an idea that which one is used to close which of these terms and these are the term which will these are your essential set of term which will arise in your these are unclosed and you close through this Lagrangian transport approach for the probability density function approach.

Now one more thing which remains there is the micro-mixing model. When we looked at the scalar PDF only thing that we talked about is the IEM.

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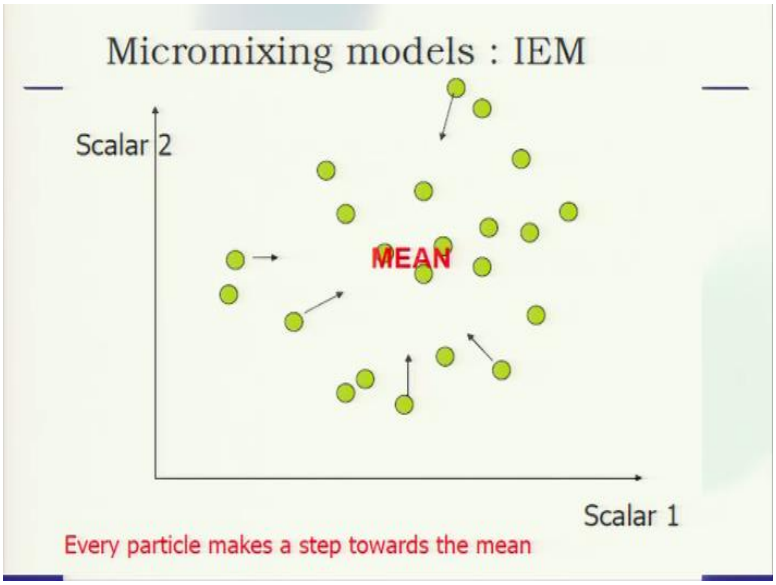

Which is essentially every particle tries to go towards the mean. This is one of the available mixing models.

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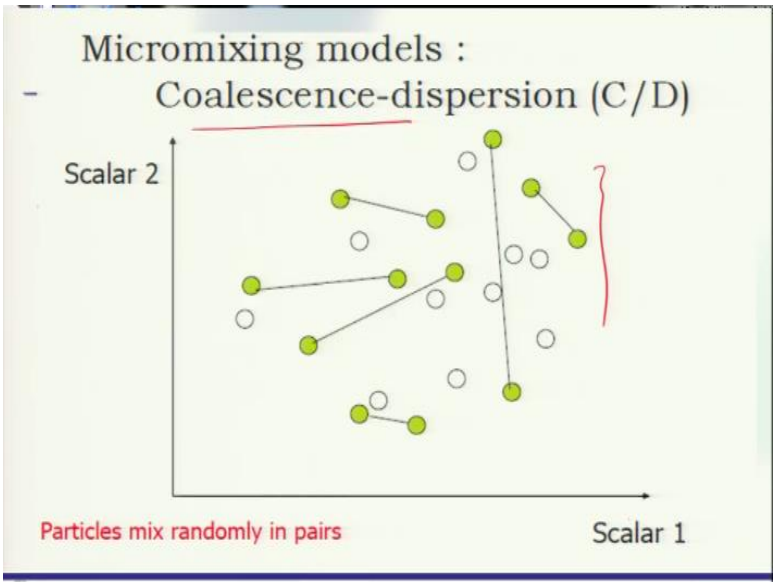

Then there are two other modal one is called the coalescences dispersion or C/D or modified C/D there are available where if this is the scalar and this direction is another scalar the particles mix randomly in pairs, this is how the mixing model works. So this is another model which is also so often available, but it depends on the flow field one can look at the impact of this different kind of mixing model or their impact on the I would say the on the results and all those things.

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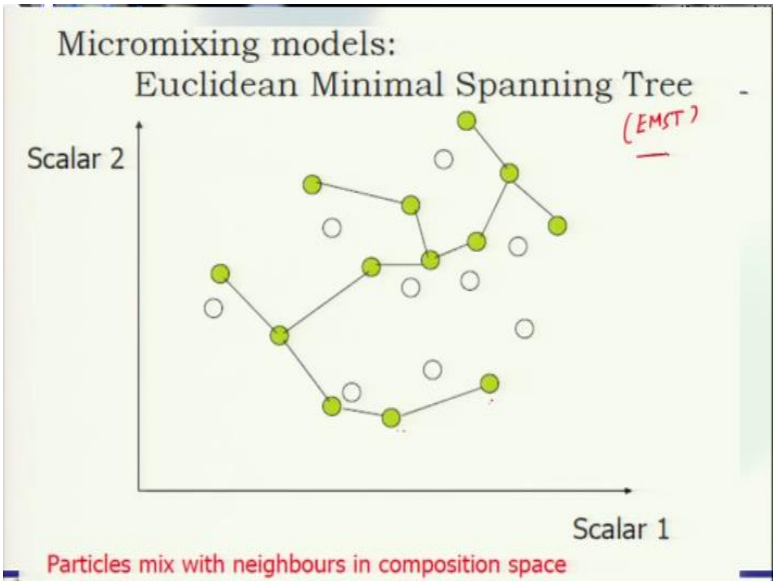

But that requires quite a bit of and the one which is quite advanced and accurate is EMST, which is called Euclidean Minimal Spanning Tree, where you what it does this particular micro- mixing model. The particles try to mix with this immediate neighbor in the composition space and then when these mix with the neighbor they will mix with this neighbor that is why they form a and that is why it is called the Euclidean spanning tree or minimum spanning tree.

So they try to I mean look at the immediate neighbor and try to pair with it which and then forms these 3, where in a larger scales that helps to find out the mixing module constant. This guy is one of the, I mean when you compare this trip particular mixing models, this is quite handy or I would say accurate compared to the to the other 2.

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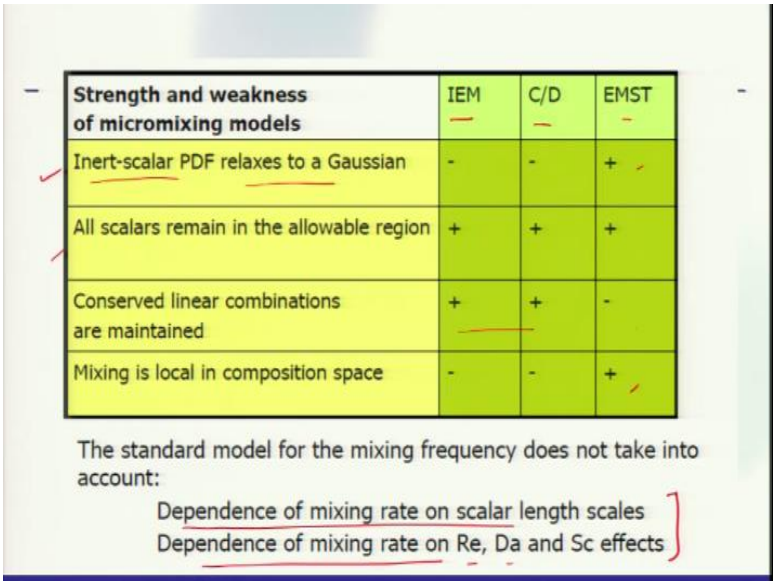

Now, obviously when say accurate still that is that remains a bit relative because when you have a particular problem or it dilutes a different kind of problems, they differ slightly. So depending on the problem to problem you have to decide upon that. Now if I just quickly put together the strength and weakness of these micro-mixing models, so there are IEM, C/D and EMST first thing the first point is inert scalar PDF will access to a Gaussian.

So this is happening in EMST only then all scalars remain in the allowable region that is true for all of them. Now the concept linear combinations are maintained, that is maintained in these 2 not here mixing is local in composition space, which is actually true for EMST. The other thing is that the standard model for this mixing frequency does not take into account. The dependence of mixing rate on scalar lens scale and dependence of mixing rate on Reynolds number Damkohler number and Smith number effect. So these are very important effect, which can be also or need to be looked at.

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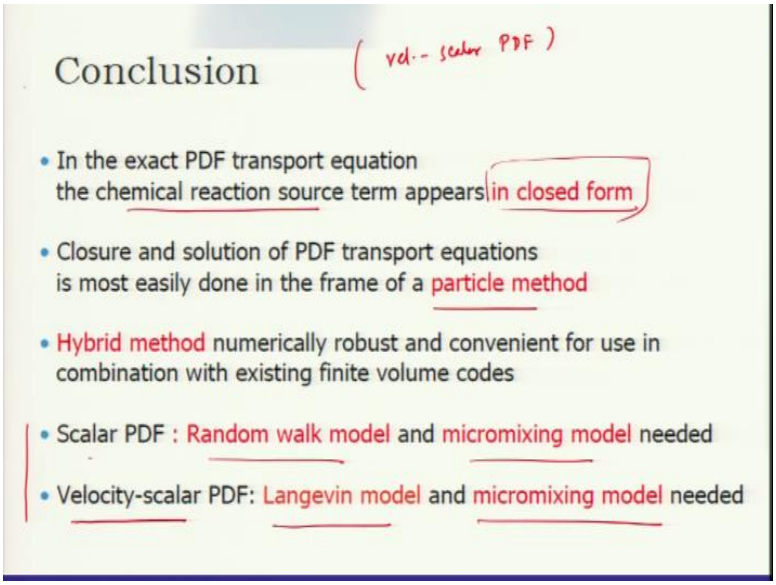

So just to sum up the things for the velocity, scalar PDF so PDF transport equation you have the chemical source term, which is one of the issues that is in closed form. So that is the biggest advantage which is true for both scalar PDF and velocities scalar PDF. Then the closure solutions of the PDF equations are usually achieved in the particle method. So the framework essentially one quality hybrid method,

Which has both the Eulerian framework and the Lagrangian framework, which is numerically quite robust and convenient for use in combination with the finite volume methods or the codes. There in scalar PDF, you have random walk model and micro-mixing model needed, where is

in velocity scalar PDF you require a Langevin model and micro mixing model, so that will close the term which are there I mean in unclosed in the system. Just to end this discussion with a simple example.

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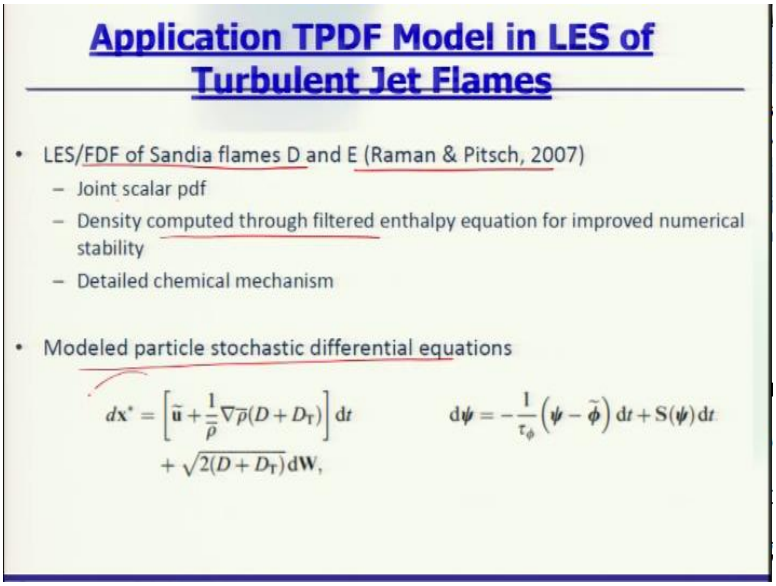

You can see this model with LES of turbulent jet flame. This was done a long time back in 2007. This is Sandia flame D where joins scalar PDF was solved which is computed through filtered enthalpy equation, chemical mechanism. So the stochastic differential equations are position and in the component.

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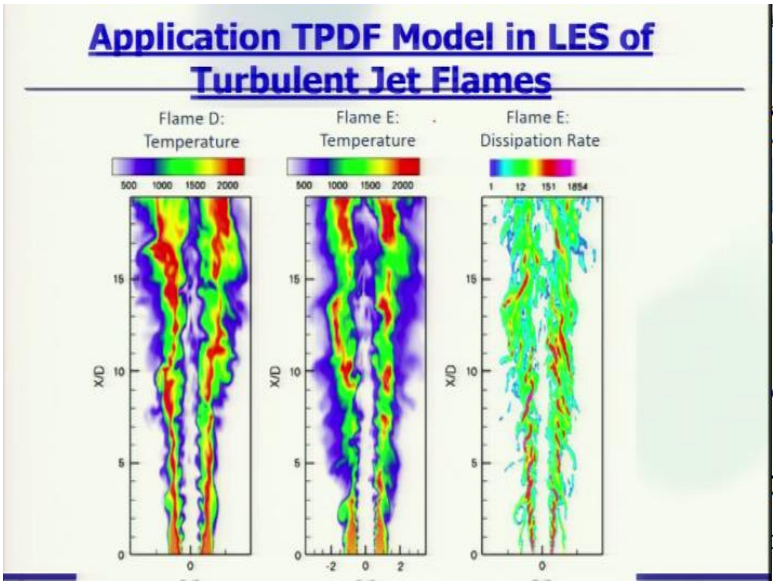

Where you can see this structure of the D, E and F for these are instantaneous structures how it looks.

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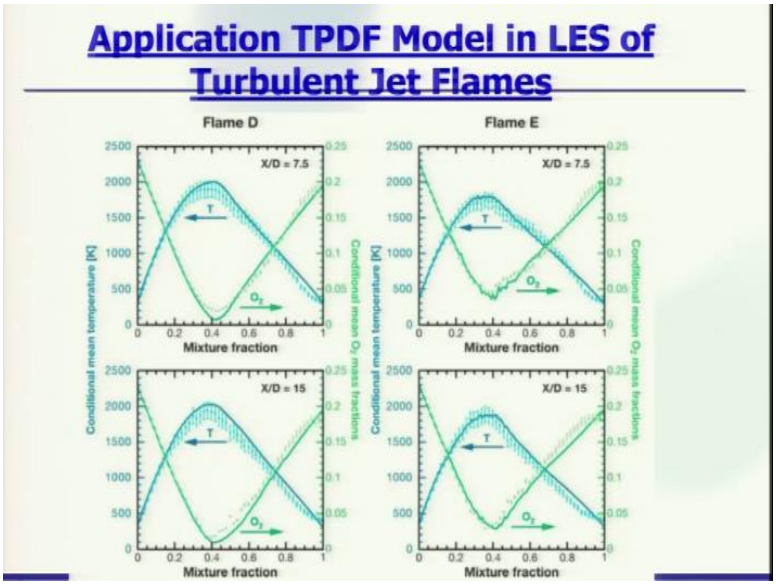

And there are mean values also, which was compared you can go to that reference and find out the rest of the detail through this is just to show you how that thing actually work and one can find out also the mean from the scatter plot so that we stopped the or essentially that concludes the discussion on the transport PDF method and we will stop the discussion today here continue in the next lecture.