

Turbulent Combustion: Theory and Modelling
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Lecture - 46
Turbulence- Chemistry Interaction (Contd.,)

Welcome back. So let us continue the discussion on the probability distribution function. So we have looked at the distribution of CDF and how we get the product distribution function, which is the derivative of CDF, and then we are now looking at the joint CDF and we stopped at the property discussion.

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Joint Cumulative Density Function

- Non-decreasing for
 $F_{1,2}(v_1 + \delta v_1, v_2 + \delta v_2) \geq F_{1,2}(v_1, v_2)$ for $\delta v_1, \delta v_2 \geq 0$
- $v_1 < -\infty$ is impossible \rightarrow
 $F_{1,2}(-\infty, v_2) = P\{v_1 < -\infty, v_2 < v_2\} = 0$
- $(v_1 < +\infty)$ is sure \rightarrow
 $F_{1,2}(+\infty, v_2) = P\{v_1 < +\infty, v_2 < v_2\} = P\{v_2 < v_2\} = F_2(v_2)$

\uparrow
 marginal CDF $\rightarrow F_1(v_1) = F_{1,2}(v_1, \infty)$

So the properties of the joint CDF,

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Joint Cumulative Density Function

- Joint PDF (jPDF)

$$f_{1,2}(v_1, v_2) = \frac{\partial^2 F_{1,2}(v_1, v_2)}{\partial v_1 \partial v_2}$$

- Fundamental property:

$$P\{v_{1a} \leq v_1 < v_{1b}, v_{2a} \leq v_2 < v_{2b}\} = \int_{v_{1a}}^{v_{1b}} \int_{v_{2a}}^{v_{2b}} f_{1,2}(v_1, v_2) dv_2 dv_1$$

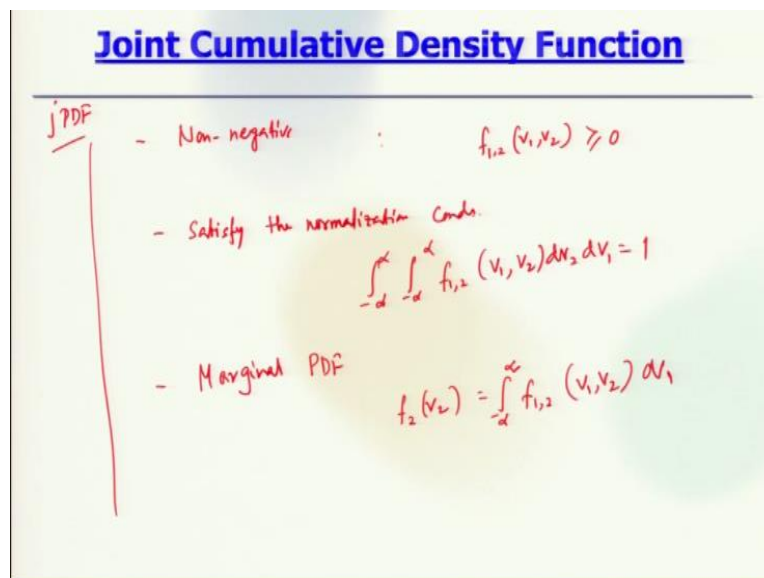
Figure 10. The v_1, v_2 sample space showing the region corresponding to the event $\{v_{1a} \leq v_1 < v_{1b}, v_{2a} \leq v_2 < v_{2b}\}$, see Eq. (10.7).

Source: Pope, "Turbulent Flows"

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Now we look at the other properties of that. That means if it is on V_1 and V_2 the joint PDF, so this would be the second derivative of this function $f_{1,2}$. So there will be one important property the fundamental properties probability of U_1 which lies between V_1 and U_2 between 2a and 2b that means this is the space. So this is how one can get, this is one of the important properties of a joint PDF function or joint.

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Now, what is jPDF? Properties that it is one thing, is that it is non-negative, that means $f_{1,2}(V_1, V_2)$ it should be greater than 0. It also satisfies the normalization, condition that means

$$\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} f_{1,2}(V_1, V_2) dv_2 dv_1 = 1$$

and marginal PDF where you get

$$f_2(v_2) = \int_{-\infty}^{+\infty} f_{1,2}(V_1, V_2) dv_1$$

So these are some of the properties of jPDF, the joint probability distribution function.

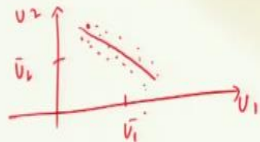
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Joint Statistics

$$Q(U_1, U_2, \dots)$$

$$Q(U_1, U_2, \dots)^n = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \dots Q(v_1, v_2, \dots)^n f_{1,2}(v_1, v_2, \dots) \dots dv_2 dv_1$$

$i = 1, 2, \dots, n > 1, \quad Q = \frac{(U_1 - \bar{U}_1)(U_2 - \bar{U}_2)}{}$

$$\overline{U_1' U_2'} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (v_1 - \bar{U}_1)(v_2 - \bar{U}_2) f_{1,2}(v_1, v_2) dv_2 dv_1$$


Now we look at the joint statistics: for let's say a function of Q where you have U₁, U₂, then the central moment, that is

$$\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} Q(v_1, v_2, \dots)^n f_{1,2}(v_1, v_2) dv_2 dv_1$$

something like that. So one can look at the example of let's say

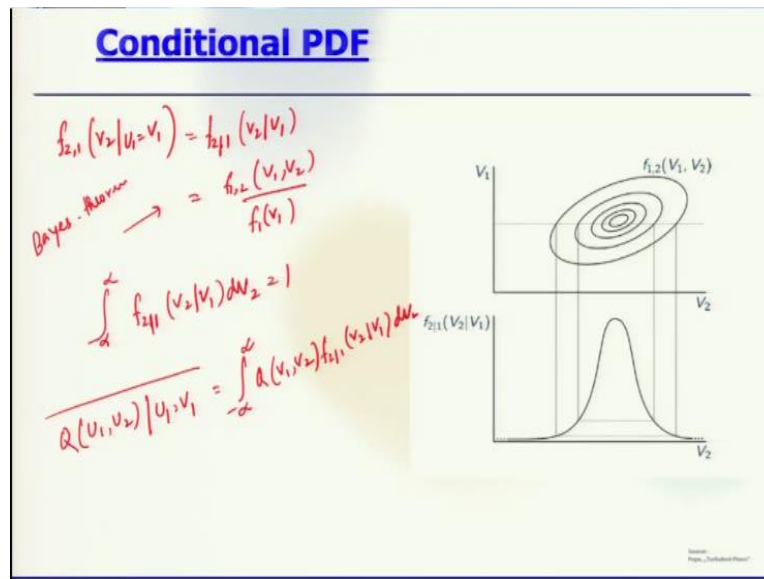
$$i = 1, 2, \quad n = 1, \quad Q = (U_1 - \bar{U}_1)(U_2 - \bar{U}_2)$$

So, the a covariance of U₁ and U₂ is

$$\overline{U_1' U_2'} = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} (v_1 - \bar{U}_1)(v_2 - \bar{U}_2) f_{1,2}(v_1, v_2) dv_2 dv_1$$

So essentially the let us say U₁, U₂ and this is \bar{U}_2 and this is \bar{U}_1 . So the mean correlation goes like that where things could be scattered in this fashion. So this actually to velocity component U₁, U₂ that is scatter plot and this is how the covariance shows the correlation between these 2 variables.

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Now if you look at the PDF of U_2 condition at $U_1 = V_1$ so that means $f_{2,1}$ where V_2 is conditioned by $U_1 = V_1$, so this would be

$$f_{2,1}(V_2|_{U_1=V_1}) = f_{2,1}(V_2|V_1)$$

So this you get from Bayes theorem.

$$= \frac{f_{1,2}(V_1, V_2)}{f_1(V_1)}$$

Now the joint PDF of $f_{1,2}$ skilled so that it satisfies the normalized condition which is

$$\int_{-\infty}^{+\infty} f_{2,1}(V_2|V_1) dV_2 = 1$$

Now

$$\overline{Q(U_1, U_2) | u_1=v_1} = \int_{-\infty}^{+\infty} Q(V_1, V_2) f_{2,1}(V_2|V_1) dV_2$$

So this is how you can see that these things. So when you have the sample space and they are conditioned on another thing.

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Statistical Independence

$$\begin{aligned} U_1, U_2 & \text{ - statistically independent} \\ f_{2|1}(v_2|v_1) & = f_2(v_2) \\ f_{2|1}(v_2|v_1) & = \frac{f_{1,2}(v_1, v_2)}{f_1(v_1)} \Rightarrow f_1(v_1) f_{2|1}(v_2|v_1) = f_{1,2}(v_1, v_2) \\ \Rightarrow f_{1,2}(v_1, v_2) & = f_1(v_1) f_2(v_2) \\ \text{- Independent variables} & \rightarrow \text{uncorrelated} \end{aligned}$$

Now one can look at the statistical description. Let us say U_1 and U_2 are statistically independent so that means

$$f_{2|1}(V_2|V_1) = f_2(V_2)$$

what one can write $f_{2|1}(V_2|V_1)$, V_1 is $f_2(V_2)$. Now Bayes theorem gives us that

$$f_{2|1}(V_2|V_1) = \frac{f_{1,2}(V_1, V_2)}{f_1(V_1)}$$

Therefore we get

$$f_1(V_1) f_{2|1}(V_2|V_1) = f_{1,2}(V_1, V_2)$$

So that means if you have an independent variable they are uncorrelated.

So in general the other one is not true, which means the uncorrelated things are not going to be always independent. So this is what you get an idea about these different terminologies in statistical.

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Turbulent Combustion Models

- Methods for reactive scalars
- Simple Models : EBU, EDM, FRCM, EDM/FRCM
- Statistical Methods: PDF, CDF,...
- Transported PDF Model
- Modeling Turbulent Premixed Combustion
 - ✓ BML-Model
 - ✓ Level Set Approach/G-equation
 - ✓ Thickened Flame/Progress Variable
- Modeling Turbulent Non-Premixed Combustion
 - ✓ Conserved Scalar Based Models
 - ✓ Flamelet-Model
 - ✓ CMC model

Now using that statistical information we look at the transport PDF-based method which is a statistical approach.

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The PDF Transport Equation Model

- pdf Transport eq. for vel. & scalars - based on one point statistics
- generic statistical description
- joint pdf transport - (Pope, 1990)

So this is similar to your moment method, so this is called the PDF Transport Equation. So we get a PDF transport equation for velocity and reactive scalars like mass fractions so this is based on 1 point statistics. Now within that framework, we can derive a generic statistical description of these turbulent reacting flows. So which will be independent of any combustion regime and then we look at the joint PDF transport equation and the scalar and that can be derived. This was proposed by Pope in 1990 and this has become quite useful in reacting system.

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The PDF Transport Equation Model

$$\begin{aligned}
 & \frac{\partial}{\partial t}(\rho P) + \nabla \cdot (\rho v P) + (\rho g - \nabla \bar{p}) \cdot \nabla_{\phi} P + \sum_{i=1}^n \frac{\partial}{\partial \psi_i} [\omega_i P] \\
 & = \nabla_{\phi} \cdot [\langle -\nabla \cdot \tau + \nabla \langle p' | v, \psi \rangle P \rangle] - \sum_{i=1}^n \frac{\partial}{\partial \psi_i} [\langle \alpha (P \Delta \nabla Y_i) | v, \psi \rangle P]
 \end{aligned}$$

∇_{ϕ} : gradient with respect to vel. components
 $\langle \dots \rangle$: Conditional mean

Now there are different ways to derive this transport equation for this joint probability density function for P is variable V and ψ which is x and t and but the discussion referring to the Pope in 2000 and 1985. So which write the convective terms in a conservative form like

$$\begin{aligned}
 & \frac{\partial}{\partial t}(\rho P) + \nabla \cdot (\rho v P) + (\rho g - \nabla \bar{p}) \cdot \nabla_{\phi} P \\
 & + \sum_{i=1}^n \frac{\partial y}{\partial \psi_i} [\omega_i P] = \nabla_v [\langle -\nabla \tau + \nabla \langle p' | v, \psi \rangle P \rangle] - \sum_{i=1}^n \frac{\partial y}{\partial \psi_i} [\omega_i P] \\
 & = \nabla_v [\langle -\nabla \tau + \nabla \langle p' | v, \psi \rangle P \rangle] - \sum_{i=1}^n \frac{\partial [\langle \nabla (P \Delta \nabla Y_i) | v, \psi \rangle P]}{\partial \psi_i}
 \end{aligned}$$

So this is the equation of the transport equation for joint probability density function which includes the velocity and the reactive scalar where ∇V is the gradient with respect to velocity components and the terms which are in within the angular brackets. These are conditional mean and similar symbol have been used for the sample space variable.

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PDF Transport Equation: Closure Problem

$$\frac{\partial(\rho P)}{\partial t} + \nabla \cdot (\rho v P) + (\rho g - \nabla \bar{p}) \cdot \nabla_v P + \sum_{i=1}^n \frac{\partial}{\partial \psi_i} [\omega_i P] =$$

$$\nabla_v \cdot [(-\nabla \cdot \tau + \nabla(p' | v, \psi) P)] - \sum_{i=1}^n \frac{\partial}{\partial \psi_i} [(\nabla \cdot (\rho D \nabla \psi_i) | v, \psi) P]$$

LHS - $\frac{D(\rho P)}{Dt}$ (1+2)

③ : transport in vel. space by gravity & mean pres. gradient

④ : chemical source term

LHS : closed form

So once we have this equation we can see this is the equation that we have written. So this is the del transient term, convection term other terms. Now the left-hand side the first 2 terms, so these 2 terms, the local change and the convection of the probability density function in physical space. So that means this will lead to the material derivative essentially of pp this 2 term will lead to that.

Then the third term which is let us say this is the first term, the second term this is the third term on the left-hand side so this is the 1 + 2. Now the third term in the left-hand side represents the transport in velocity space by gravity and mean, pressure, gradient and this is the last term which is the fourth term. So the fourth term on the left-hand side is a chemical source term. Now if you look at all these terms on the left-hand side, they are all in closed form.

So on the left-hand side, there is nothing because they are closed form. They are all local in physical space. So left-hand side you see there is no unclose term, now while we move to the other side.

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PDF Transport Equation: Closure Problem

Note: - mean pres. gradient → does not present a closure problem

Reacting syst - Chem. source term needs to be treated exactly

Now another thing one can note is that the mean, pressure, the gradient does not present the closer problem since the pressure is calculated independent of the PDF equation using the mean velocity field. Also, so that means you can mean, pressure, gradient so this does not present a closer problem since the pressure is calculated independently of the PDF so for reacting system.

The chemical source term needs to be treated exactly or properly. Now always there has been an argument that respects to the transport PDF formulation. It has a considerable advantage over other formulations. But we can see what are those things?

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PDF Transport Equation: Closure Problem

$$\frac{\partial(\rho P)}{\partial t} + \nabla \cdot (\rho v P) + (\rho g - \nabla \bar{p}) \cdot \nabla_v P + \sum_{i=1}^n \frac{\partial}{\partial \psi_i} [\omega_i P] =$$

$$\nabla_v \cdot \left[\underbrace{(-\nabla \cdot \tau + \nabla(p' |v, \psi) P)}_{(1)} \right] - \sum_{i=1}^n \frac{\partial}{\partial \psi_i} \left[\underbrace{(\nabla \cdot (\rho D \nabla \psi_i) |v, \psi) P}_{(2)} \right]$$

- if gradients are not included as sample space → these need closure

Now, look at the right-hand side of that equation. So there are 2 terms on the right-hand side term, this is first and this is the second term. So, these terms on the right-hand side, contain the gradient of quantities condition on values of velocity and composition. So the gradients are not

included as sample space, so the, if gradients are not included as sample space variable in PDF equation these terms would arise as an unclosed term and needs modeling.

So there are issues one has to be careful here. These terms are actually content gradient because they are all and the gradient and also conditioned on velocity and scalar field. If the gradients are not part of our sample space then these need closure, so one has to close this term properly.

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PDF Transport Equation: Closure Problem

$$\frac{\partial(\rho P)}{\partial t} + \nabla \cdot (\rho v P) + (\rho g - \nabla \bar{p}) \cdot \nabla_v P + \sum_{i=1}^n \frac{\partial}{\partial \psi_i} [\omega_i P] =$$

$$\nabla_v \cdot \left[\underbrace{(-\nabla \cdot \tau + \nabla \langle p' | v, \psi \rangle P)}_{\textcircled{1}} \right] - \sum_{i=1}^n \frac{\partial}{\partial \psi_i} \left[\underbrace{(\nabla \cdot (\rho D \nabla \psi_i)) | v, \psi \rangle P}_{\textcircled{2}} \right]$$

① - Transport of the pdf in vel. space induced by the viscous stresses and the fluctuating pres. gradient

② Transport in reactive scalar space by molecular fluxes → molec

Now the first term and the second term on the right-hand side. The first term is an unclosure term on the right-hand side it described the transport of the PDF in velocity space induced by the viscous stresses and the fluctuating pressure gradient. So the second term represents the transport in reactive scalar space or in the composition face by molecular fluxes, so this essentially leads to the or it represents molecular mixing.

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PDF Transport Equation: Closure Problem



When the chemistry is first mixing and reaction take place in thin layers, so chemistry fasts the mixing and reaction take place in thin layers so that molecular transport and the chemical source term balance each other. So the closed chemical source term and unclosure molecular mixing term being leading order terms in the asymptotic description. So the right-hand sides there are terms that are in asymptotic distribution the flame structure and closed will link to each other.

Now, this has been already illustrated by Pope in 1984 the case of pre-mixed combustion when we compare a standard PDF closer for molecular mixing and with the molecular mixing term with the formulation so the molecular diffusion term was combined with the chemical source term to define a modified reaction rate. So there is the one distributed combustion on the generate combustion find considerable differences in Damkohler number dependencies. So there are some issues that are there, now how do you get a solution for the PDF equation?

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PDF Transport Equation: Solution

- ❖ From a **numerical point of view**, the most apparent property of the pdf transport equation is its **high dimensionality**
- ❖ Finite-volume and finite-difference techniques are not very attractive for this type of problem, as memory requirements increase roughly exponentially with dimensionality
- ❖ Therefore, virtually all numerical implementations of pdf methods for turbulent reactive flows employ **Monte-Carlo simulation techniques** (cf. Pope, 1981, 1985)
- ❖ The advantage of Monte-Carlo methods is that their memory requirements depend only linearly on the dimensionality of the problem

Now from a numerical point of view, the most apparent property of the PDF transports its high dimensionality it is a highly dimensional, that is why typical your computational technique like finite volume or finite difference kind of techniques are not very attractive for this type of problem. Why? Because the memory requirements increase with the dimensionality.

So the virtually all numerical implementation of this kind of methods are using Monte - Carlo kind of techniques, which are particle-based method and the advantage is that memory requirement is not that much and it is also can handle this high dimensional problem.

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PDF Transport Equation: Solution

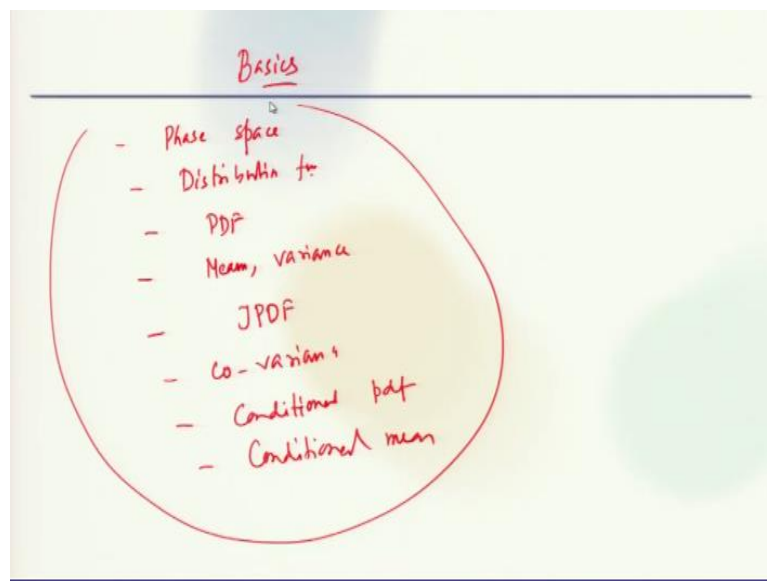
- Monte-Carlo methods employ a large number, N , of so called notional particles (Pope, 1985)
- Particles should be considered different realizations of the turbulent reactive flow problem under investigation
- Particles should not be confused with real fluid elements, which behave similarly in a number of respects
- Statistical error decreases with $N^{1/2}$
-Slow convergence

So these also use some large number of particles, this is called notional particles. So, that means now so far our discussion, if you look at the governing equation of the PDF transport equation, which is in a physical space in the eulerian framework. Now, when you try to solve this

particular equation, we are moving to a situation where we are introducing particles that mean it is in lagrangian framework.

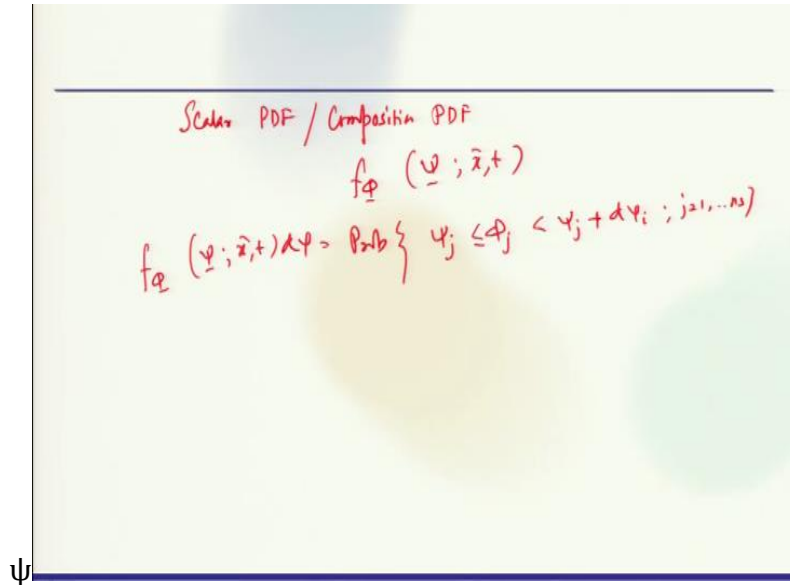
Now the particles should be considered different realizations of the turbulent reacting problem under this investigation. It should not be confused with the real fluid element and the statistical error and all these things also decrease with a number of particles. Obviously there have been issue with the convergence because once you have the high dimensional problem with large number of particles, these are obvious.

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Now we can look at some of the basics from statistics 1 is the phase space which we have already looked at the distribution, function, probability density function, mean, variance, joint PDF, co-variance, conditional PDF and conditional mean. So these are some of the properties which will be used and we have already now.

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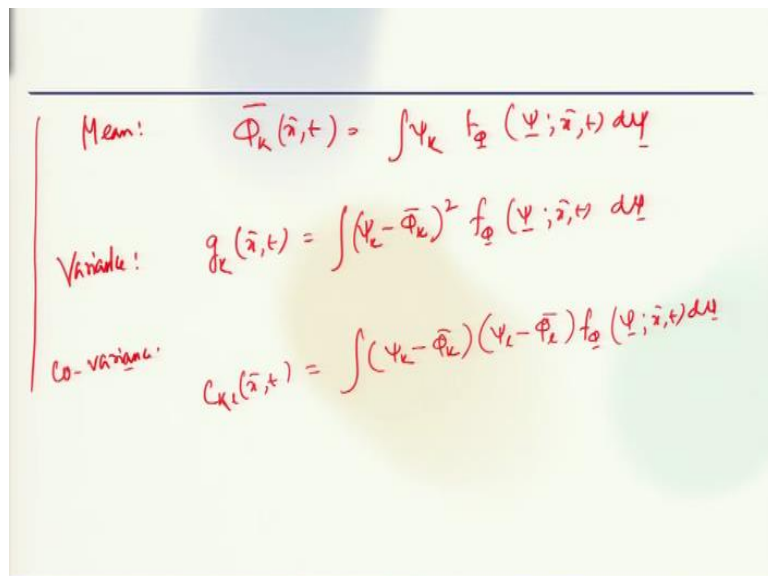


Now, one can find out the one point probability density function, which is the scalar PDF or composition PDF which is defined at $f_\phi(\psi; \bar{x}, t)$. So

$$f_\phi(\psi; \bar{x}, t) d\psi = Prob\{\psi_j \le \phi_j < \psi_j + d\psi_j; j = 1, \dots, n_s\}$$

So in stationary combustion system, the PDF is time independent and we can find out the mean.

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So the mean would be

$$\phi_k(\bar{x}, t) = \int \psi_k f_\phi(\psi, \bar{x}, t) d\psi$$

and variance one can find out the variance which would be

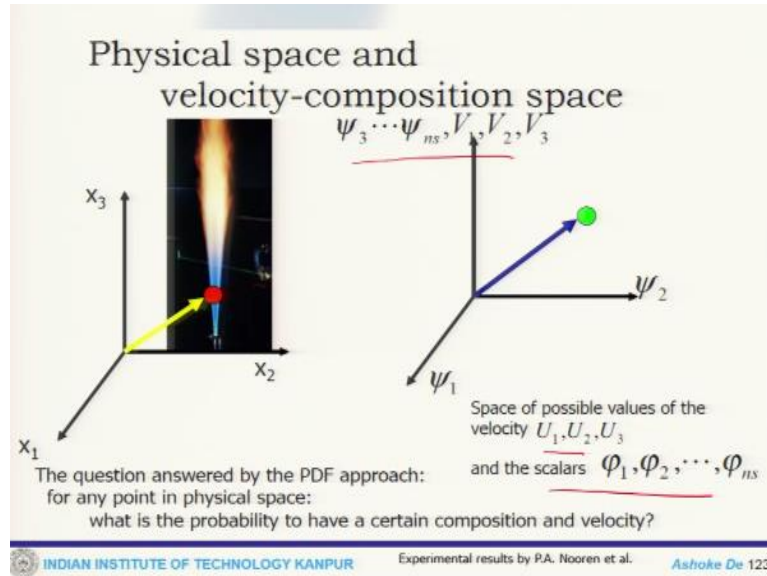
$$g_k(\bar{x}, t) = \int (\psi_k - \bar{\phi}_k)^2 f_\phi(\psi, \bar{x}, t) d\psi$$

and the covariance is

$$C_{kl}(\bar{x}, t) = \int (\psi_k - \bar{\phi}_k)(\psi_l - \bar{\phi}_l) f_\phi(\psi, \bar{x}, t) d\psi$$

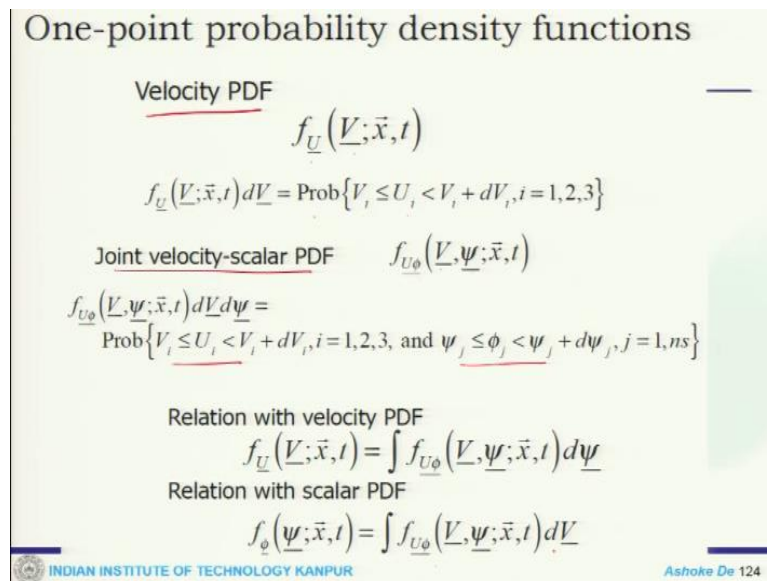
This is how from the distribution of the composition PDF you can find out this mean, variance and covariance.

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Now if we look at the physical space problem is here and we transform the velocity composition PDF, that means you have 3 velocity component variable and the scalar variable so they will form these total space which is a joint velocity composition period and one can see what is the probability to have certain compositions over there.

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Now if you look at the one point for the density function, so the only velocity PDF you can write this is the velocity so the probability of some samples the line between these 2

components that is the probability of that. Now the joint velocity scalar PDF so it will be both on U and Φ so this is velocity and scalars and the probability of finding an event would be between a velocity component and the scalar component.

So now one can correlate the velocity PDF to so the velocity pure velocity PDF can be obtained from the joint velocities scalar PDF when you integrate over the side and the scalar PDF can be obtained when the joint PDF we took an integration over velocity variable.

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**One-point probability density functions
for density weighted quantities**

Joint velocity-scalar PDF

$$\tilde{f}_{U\phi}(\underline{U}, \underline{\psi}; \bar{x}, t) = \frac{\rho(\underline{\psi})}{\bar{\rho}} f_{U\phi}(\underline{U}, \underline{\psi}; \bar{x}, t)$$

Scalar PDF, or composition PDF

$$\tilde{f}_{\phi}(\underline{\psi}; \bar{x}, t) = \frac{\rho(\underline{\psi})}{\bar{\rho}} f_{\phi}(\underline{\psi}; \bar{x}, t)$$

Now, we can look at this one-point PDF for density-weighted quantities because this is very important we have already seen that if we are dealing with the reacting system this density-weighted average is quite handy to avoid all these density fluctuations that arise during averaging. So now similarly for the joint velocities scalar PDF, this would be the density-weighted quantities and one can write rho psi by rho bar with this and for scalar PDF or composition PDF, this would be written like this.

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Exact equations for mean properties
contain unclosed terms

$$\frac{\partial}{\partial t}(\bar{\rho}) + \frac{\partial}{\partial x_i}(\bar{\rho} \bar{u}_i) = 0$$

$$\frac{\partial}{\partial t}(\bar{\rho} \bar{u}_j) + \frac{\partial}{\partial x_i}(\bar{\rho} \bar{u}_i \bar{u}_j) = \left[-\frac{\partial \bar{p}}{\partial x_j} + \frac{\partial \bar{\tau}_{ij}}{\partial x_i} + \bar{\rho} g_j \right] - \frac{\partial}{\partial x_i}(\bar{\rho} \widetilde{u_i u_j}) \quad \text{1}$$

Reynolds stress

$$\frac{\partial}{\partial t}(\bar{\rho} \bar{\phi}_k) + \frac{\partial}{\partial x_i}(\bar{\rho} \bar{\phi}_k \bar{u}_i) = \left[-\frac{\partial}{\partial x_i}(\bar{J}_i^k) + \bar{\rho} \bar{S}_k \right] - \frac{\partial}{\partial x_i}(\bar{\rho} \widetilde{\phi_k u_i}) \quad \text{2}$$

Mean source term Turbulent scalar flux

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So now again coming back to our equations, this is our continuity equation, this is our momentum equation where we will get Reynolds stress or scalar transport equation will have source term and turbulence scalar flux.

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Closure using the velocity-scalar PDF

Reynolds stress tensor

$$\text{1} \quad \bar{\rho} \widetilde{u_i u_j} = \overline{\rho u_i u_j} \equiv \bar{\rho} \int (V_i - \bar{U}_i)(V_j - \bar{U}_j) \tilde{f}_{\underline{V}}(\underline{V}; \bar{x}, t) d\underline{V}$$

Turbulent scalar flux

$$\text{2} \quad \bar{\rho} \widetilde{\phi_k u_j} = \overline{\rho \phi_k u_j} \equiv \bar{\rho} \int (\psi_k - \bar{\phi}_k)(V_j - \bar{U}_j) \tilde{f}_{\underline{V}, \underline{\psi}}(\underline{V}, \underline{\psi}; \bar{x}, t) d\underline{V} d\underline{\psi}$$

Mean source term

$$\text{3} \quad \bar{\rho} \bar{S}_k = \overline{\rho S_k} \equiv \bar{\rho} \int S_k(\underline{\psi}) \tilde{f}_{\underline{\psi}}(\underline{\psi}; \bar{x}, t) d\underline{\psi}$$

Now, these are a set of governing equations and how we close that Reynolds stress using some RANS-based model, turbulence scalar flux, so you can use gradient assumption and source term, the mean source term now we can close using composition PDF method. So this is now the difference that we see when we are talking about other models compared to transport PDF-based model and similar things one can close it using velocity scalar joint PDF.

So this is Reynolds stress term, which could be using the joint PDF or velocity PDF one can close it. So instead of taking it directly from the RANS equation now, we can use the lagrangian

information to close its turbulence scalar flux, which is this term now we can close it using both velocity scalar joint PDF and source term using the scalar product. So that means all these closures are now done using the probability distribution function.

So this is a substantial difference when one looks at the flow field in the pollen framework and when one looks at the Lagrangian framework in the context of the transport PDF equation, so we will stop the discussion here today and continue the discussion in the next lecture.