On discrete representation of filtered density functions for turbulent combustion

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1. Motivation and objectives

Following the success of transported probability density function (PDF) methods (Pope 1985) in a Reynolds-averaged Navier-Stokes (RANS) context, the transported PDF concept in the context of Large-Eddy Simulations (LES) has become increasingly popular in the simulations of turbulent reacting flows. First suggested by Givi (1989), the application of the transported PDF method to LES started, however, only after the concept of Filtered Density Function (FDF) was introduced as a LES analog of PDF (Pope 1990). Based on this FDF concept, transported FDF methods for LES have been developed (Gao & O'Brien 1993; Colucci *et al.* 1998; Jaberi *et al.* 1999; Gicquel *et al.* 2002; Sheikhi *et al.* 2003; Raman *et al.* 2006). The developments have been reviewed and recent results and prospects discussed (Givi 2006). It is promising that transported FDF methods will become effective and powerful in the predictive simulations of turbulent combustion using LES.

Like the application to LES of other turbulent combustion models developed for RANS (Pitsch 2006), there are fundamental differences between transported PDF methods and transported FDF methods. However, these differences are not fully addressed in the current implementations of the transported FDF method. Because of the same high dimensionality of FDF as that of PDF, it is typical to employ the Lagrangian Monte Carlo scheme (Pope 1994) for the solution of the transport FDF equation and the FDF is represented in the same way as the PDF by an ensemble of particles. In the PDF method these particles contain values from different realizations of the flow and how the ensemble represents the PDF has been shown (Pope 1994); in the FDF method these are open questions. Furthermore, current FDF particle implementations make reference to the principle of stochastically equivalent systems (Pope 1985); in the PDF method this principle is applied to the stochastic and fluid particles systems. The stochastic models are able to determine Eulerian PDFs and means is because the Lagrangian PDF (defined for Lagrangian particles) is the transition density and determines the transition of the Eulerian PDF from time t_0 to time t (Pope 1994). However, in the FDF method it is unclear how a Lagrangian FDF can be defined since FDF involves spatial filtering and a Lagrangian particle represents one spatial point. It is unclear how the stochastic particle system determines the FDF that is Eulerian by nature. In addition, for turbulent reacting flow the appropriate design of a mixing model is essential for the performance of the FDF method; current FDF implementations commonly employ the IEM (interaction by exchange with mean) mixing model, which is known to violate the physics of mixing (Subramaniam & Pope 1998). These issues need to be resolved for the future development of the transported FDF method.

The fundamental difference between FDF and the PDF developed in the RANS context is that in RANS, mean quantities are sought and the PDF (RANS PDF, for clarity) is used to characterize fluctuations over different flow realizations. In LES, instantaneous filtered quantities are sought and the FDF is used to characterize the instantaneous subfilter fluctuations. The relationship between the two is that in the limit of the filter width goes to zero the mean of FDF is the RANS PDF (Pope 1990). Following the same line of thinking as the RANS PDF, a LES PDF is proposed to describe the subfilter fluctuations as a true conditional PDF defined on the sub-ensemble of all realizations of the turbulent flows that have the same filtered field (Fox 2003). Similarly, a filter PDF is discussed as the average of the FDF of many flow realizations and arguments are made that one cannot model based on the FDF because the models are statistical in nature and the filter PDF is required for modeling (Pitsch 2006). These LES PDFs that are based on different flow realizations might be alternatives for LES subfilter modeling, but they complicate the conceptual issues in the development of transported PDF method for LES.

In spite of the difference between the FDF and RANS PDF, however, it has been noted (Gao & O'Brien 1993; Pope 2000) that the FDF has all the properties of a mathematical PDF. The nature of this mathematical PDF has never been described, and this is probably the source of those unresolved issues when transported FDF methods employ the solution schemes that have been developed for the RANS PDF.

The purpose of this paper is to offer two different lines of thinking: (1) a transported FDF method can directly use the property of fine-grained PDF (Pope 2000) from the definition of the FDF; and (2) unlike the RANS PDF, a PDF can be defined from one realization of the turbulent flow. If statistical samples are taken in the vicinity of a spatial point in a turbulent flow at one instance of time to represent the flow properties at that spatial point, an ensemble of random values is obtained and a PDF can be used to characterize this source of randomness. If the samples are taken in a way that is restricted by the filter function, then this PDF is the same as the FDF. These perspectives have some advantages and some unresolved issues can be reinterpreted and clarified.

This paper is organized as follows: the discrete/particle representation of the RANS PDF is first described to serve as a reference for the understanding of the issues in FDF methods. Then two ways of discretely representing FDF are discussed; the second is based on the fact that FDF is a mathematical PDF. This fact is first discussed conceptually and then shown mathematically. A method of calculating the FDF from DNS data is then proposed. In addition, the conditional filtered quantities are defined in terms of conditional averages that have been rigorously established. After these considerations, an original discrete representation of FDF is proposed for filtered mass density functions defined for variable density flows. This representation is different from those currently used in the solution of transported FDF equation. The modeling principle for the solution of the transport FDF equation,which has been derived in terms of subfilter PDF interpretation, is then discussed and proposed. In the last section, a mixing model is proposed that naturally satisfies the locality criterion and is more physics-based.

2. Discrete representation of PDF

In transported PDF methods, discrete, or particle, representations of the PDF play an important role in the solution and modeling of the PDF transport equations, and are often expressed in terms of Dirac delta functions. Using the sifting property of the delta function, the PDF of a scalar can be written as

$$PDF = f_\phi(\psi; \boldsymbol{x}, t) = \int_{-\infty}^{\infty} \delta(\psi - \phi) f(\phi; \boldsymbol{x}, t) \mathrm{d}\phi. \tag{2.1}$$

Here one scalar is considered for simplicity and the extension to joint PDFs of multiple scalars is straightforward. The semicolon notation indicates that f_ϕ is a density with respect to ϕ and can vary with space ($\boldsymbol{x}$) and time (t). Equation 2.1 can be interpreted as the expectation of the δ function (Pope 1985). In practice there are several ways to approximate mathematical expectations including ensemble average. Using ensemble average, Eq. 2.1 can be approximated as

$$f(\psi;\boldsymbol{x},t) \approx f_{\phi N}(\psi;\boldsymbol{x},t) = \frac{1}{N}\sum_{n=1}^{N}\delta[\psi - \phi^n(\boldsymbol{x},t)], \tag{2.2}$$

if N is large enough. This is the discrete representation (approximation) of the RANS PDF; the question of how $f_{\phi N}(\psi;\boldsymbol{x},t)$ represents $f(\psi;\boldsymbol{x},t)$ has been discussed by Pope (1994). Note that in Eq. 2.2 ϕ^n are taken from the same spatial location and time of different flow realizations. It has been shown that this discrete representation is the normalized sample point number density in the sample (ψ) space (Pope 1985). Note also that ϕ^n, the discrete PDF particles, are the samples of a random variable with PDF $f(\psi;\boldsymbol{x},t)$. In a simulation, the statistical distribution of ϕ^n is enforced by evolving ϕ^n according to the transport equation of $f(\psi;\boldsymbol{x},t)$, and this evolution is carried out through stochastic processes that model the transport equation of $f(\psi;\boldsymbol{x},t)$.

3. Discrete representation of FDF

In the application of the PDF method to LES, the filtered density function (FDF) is defined directly in terms of the delta function (Pope 1990):

$$FDF = F_\phi(\psi;\boldsymbol{x},t) = \int_{-\infty}^{+\infty}\delta[\psi - \phi(\boldsymbol{r},t)]G(|\boldsymbol{x}-\boldsymbol{r}|)\mathrm{d}\boldsymbol{r}, \tag{3.1}$$

where G is the localized, spatially and temporally invariant filter function that satisfies

$$G(\boldsymbol{x}) \geq 0, \quad G(\boldsymbol{x}) = G(-\boldsymbol{x}), \quad \text{and} \int_{-\infty}^{+\infty} G(\boldsymbol{x})\mathrm{d}\boldsymbol{x} = 1. \tag{3.2}$$

In the above equations, abbreviated notations have been used, for example, an infinitesimal volume in physical $\boldsymbol{x}$ space is written d$\boldsymbol{r}$ and a single integral sign represents integration over the whole of $\boldsymbol{x}$ space. Equation 3.1 shows that by definition FDF is the spatial (and localized) average of the delta function with G being the weight.

There can be two ways to approximate, or discretely represent, FDF. The first way is the numerical integration of Eq. 3.1:

$$F_\phi(\psi;\boldsymbol{x},t) \approx F_{\phi N}(\psi;\boldsymbol{x},t) = \sum_{n=1}^{N}\delta[\psi - \phi(\boldsymbol{r^n},t)]G(|\boldsymbol{x}-\boldsymbol{r^n}|)\triangle V, \tag{3.3}$$

where $\triangle V = V/N$ and V is the volume of the space where $G(\boldsymbol{x}) > 0$. If the common box filter is used, then

$$F_{\phi N}(\psi;\boldsymbol{x},t) = \frac{1}{N}\sum_{n=1}^{N}\delta[\psi - \phi(\boldsymbol{r^n},t)]. \tag{3.4}$$

This representation looks similar to the one for the RANS PDF (Eq. 2.2), but the significant difference is that $\phi(\boldsymbol{r^n},t)$ are taken from different spatial locations within the filter volume and from one flow realization. If the transport equation for the scalar ϕ is written as

$$\frac{\partial \rho\phi}{\partial t} + \frac{\partial \rho u_i \phi}{\partial x_i} = -\frac{\partial J_i^{\phi}}{\partial x_i} + \rho S_{\phi}, \tag{3.5}$$

a transport equation for the delta function $\delta[\psi - \phi(\boldsymbol{r^n}, t)]$, or the fine-grained PDF, may be derived as (Pope 2000):

$$\frac{\partial \rho\delta}{\partial t} + \frac{\partial u_i \rho\delta}{\partial x_i} = \frac{\partial}{\partial \psi}\left[\frac{1}{\rho}\frac{\partial J_i^{\phi}}{\partial x_i}\rho\delta\right] - \frac{\partial}{\partial \psi}\left[S_{\phi}\rho\delta\right]. \tag{3.6}$$

This equation can be the first step in the derivation of the (RANS) PDF transport equation (taking the mean operation), or in the derivation of the FDF transport equation (taking the filtering operation). A stochastic particle system may be constructed to solve this equation. However, besides a model for the molecular mixing term, the instantaneous velocity at location $\boldsymbol{r}$ needs to be constructed using the filtered velocity at location $\boldsymbol{x}$ and a model for the subfilter fluctuations.

Another way to discretely represent FDF is apparent when FDF is shown to be the PDF of subfilter scalar variables (FPDF). This FPDF is different from the RANS PDF because it is constructed from one realization of the flow. Let's consider the randomness that occurs when we try to pick a scalar value within a subfilter volume centered at a spatial point $\boldsymbol{x}$ to represent the value at that point on one flow realization. The ensemble of samples to define the FPDF is then considered as follows: first, a statistical experiment is conducted to sample spatial locations with a PDF of G, the filter function, and the scalar values (or any flow properties) at those locations are taken as the outcomes of this experiment; then a random variable can be defined to represent these outcomes and a PDF can be constructed to describe the probability distribution of this random variable. Therefore, the source of randomness to define the FPDF comes from the random fluctuations in the subfilter volume on one flow realization and is weighted by the filter function G.

Mathematically, this FPDF can be constructed from considering the filtered value of function $Q[\phi(\boldsymbol{r}, t)]$

$$\overline{Q(\boldsymbol{x}, t)} = \int_{-\infty}^{+\infty} Q[\phi(\boldsymbol{r}, t)]G(|\boldsymbol{x} - \boldsymbol{r}|)d\boldsymbol{r}. \tag{3.7}$$

Since Q is a function of $\boldsymbol{r}$, this equation can be interpreted as the local spatial average, or a mathematical expectation, of Q with G being the PDF of $\boldsymbol{r}$. Indeed, the filter function G has all the properties of a PDF. Since Q is also a function of ϕ, whose local statistics determine the local statistics of Q, we can rewrite the expectation in Eq. 3.7 in terms of the PDF of $\phi(\boldsymbol{r}, t)$, which is valid within the subfilter volume,

$$\overline{Q(\boldsymbol{x}, t)} = \int_{-\infty}^{+\infty} Q(\psi)f(\psi; \boldsymbol{x}, t)d\psi. \tag{3.8}$$

Note that this subfilter PDF, $f(\psi; \boldsymbol{x}, t)$, will be different on different flow realizations, while the RANS PDF in transported PDF method is the same on different flow realizations. In terms of the sifting property of the delta function, this subfilter PDF can be written as

$$f(\psi; \boldsymbol{x}, t) = \int_{-\infty}^{+\infty} \delta(\psi - \phi)f(\phi; \boldsymbol{x}, t)d\phi. \tag{3.9}$$

This is the expectation of the delta function within the subfilter volume. Since ϕ in the delta function corresponds to the values at different $\boldsymbol{r}$ locations and Eqs. 3.7 and 3.8 state that the filtering operation, multiplying by G and then integrating over physical space $\boldsymbol{r}$, is equivalent to the local mean operation, i.e., multiplying by the subfilter PDF (or FPDF) and then integrating over the sample space ψ, the expectation of the delta function in Eq. 3.9 can be expressed in terms of the PDF of $\boldsymbol{r}$,

$$f(\psi;\boldsymbol{x},t) = \int_{-\infty}^{+\infty} \delta[\psi - \phi(\boldsymbol{r},t)]G(|\boldsymbol{x}-\boldsymbol{r}|)d\boldsymbol{r} = F_\phi(\psi;\boldsymbol{x},t). \tag{3.10}$$

It is hence shown that the FPDF of ϕ within the subfilter volume centered at $\boldsymbol{x}$ is the FDF of ϕ at $\boldsymbol{x}$. In addition, the property that filtering operation is equivalent to the local averaging operation using FPDF/FDF can be used in the derivation of the FDF transport equation, as shown in the following.

This FPDF interpretation of FDF suggests a way of evaluating the FDF from direct numerical simulation (DNS) data. For example, suppose that there are N_d DNS cells within the subfilter volume of interest and the box filter is to be used, then

$$F_\phi(\psi;\boldsymbol{x},t)\triangle\psi \approx \frac{\sum_{i=1}^{N_\psi} V_i}{\sum_{n=1}^{N_d} V_n}, \tag{3.11}$$

where V_n are the volumes of the DNS cells, N_ψ is the number of cells within which the scalar values are in the range $\psi \leq \phi < \psi + \triangle\psi$, and $\triangle\psi$ is a small increment in the sample space. The specification of $\triangle\psi$ and how to calculate the volume within the range of $\psi \leq \phi < \psi + \triangle\psi$ (instead of using the simple sum for the numerator in Eq. 3.11) determine the accuracy of this approximation.

If a filter function other than the box filter is to be used, a transformation of the physical volume may be introduced

$$v(\boldsymbol{r}) = \int_{-\infty}^{\boldsymbol{r}} G(|\boldsymbol{y}|)d\boldsymbol{y}, \quad \text{such that } dv = Gd\boldsymbol{r}. \tag{3.12}$$

Since the filtering operation after the transformation becomes

$$\overline{Q(\boldsymbol{x},t)} = \int_0^1 Q[\phi(v;\boldsymbol{x},t)]dv, \tag{3.13}$$

Eq. 3.11 can then be applied in the v space instead of the physical space.

With the FPDF view of the FDF, the conditional filtered values can be interpreted as the local conditional expectations that have been treated rigorously in PDF method (Pope 2000). For example, suppose that u is another subfilter variable and the joint FDF of u and ϕ is

$$F_{u\phi}(V,\psi;\boldsymbol{x},t) = \int_{-\infty}^{+\infty} \delta[V - u(\boldsymbol{r},t)]\delta[\psi - \phi(\boldsymbol{r},t)]G(|\boldsymbol{x}-\boldsymbol{r}|)d\boldsymbol{r}. \tag{3.14}$$

Since FDFs are FPDFs, a conditional FDF may be interpreted as a conditional PDF, i.e., using Eq. 2.145 in Pope (1985), the conditional FDF $F_{u|\phi}(V|\psi)$ can be written as

$$F_{u|\phi}(V|\psi;\boldsymbol{x},t) = \frac{F_{u\phi}(V,\psi;\boldsymbol{x},t)}{F_\phi(\psi;\boldsymbol{x},t)} = \frac{\int_{-\infty}^{+\infty} \delta[V - u(\boldsymbol{r},t)]\delta[\psi - \phi(\boldsymbol{r},t)]G(|\boldsymbol{x}-\boldsymbol{r}|)d\boldsymbol{r}}{\int_{-\infty}^{+\infty} \delta[\psi - \phi(\boldsymbol{r},t)]G(|\boldsymbol{x}-\boldsymbol{r}|)d\boldsymbol{r}}. \tag{3.15}$$

The local conditional expectation of $u(\boldsymbol{x},t)$, which can be expressed as using Eq. 3.15

$$\mathrm{E}(u(\boldsymbol{x},t)|\phi=\psi)=\int_{-\infty}^{+\infty} VF_{u|\phi}(V|\psi;\boldsymbol{x},t)dV=\frac{\int_{-\infty}^{+\infty} u(\boldsymbol{r},t)\delta[\psi-\phi(\boldsymbol{r},t)]G(|\boldsymbol{x}-\boldsymbol{r}|)d\boldsymbol{r}}{F_\phi(\psi;\boldsymbol{x},t)}, \tag{3.16}$$

can be interpreted as conditional filtered value of $u(\boldsymbol{x},t)$, i.e., $\overline{u(\boldsymbol{x},t)|\phi=\psi}$. This is the same expression for conditional filtered values that has been defined during the derivation of transport FDF equations (Gao & O'Brien 1993; Colucci *et al.* 1998; Jaberi *et al.* 1999; Gicquel *et al.* 2002; Sheikhi *et al.* 2003).

Having established that the FDF is the PDF of the subfilter variables, we can express the FDF as the expectation of the delta function in the same manner as in Eq. 2.1:

$$F_\phi(\psi;\boldsymbol{x},t)=\int_{-\infty}^{\infty}\delta(\psi-\phi)F(\phi;\boldsymbol{x},t)d\phi, \tag{3.17}$$

and we can approximate this expectation in terms of the ensemble average

$$F_\phi(\psi;\boldsymbol{x},t)\approx F_{\phi N}(\psi;\boldsymbol{x},t)=\frac{1}{N}\sum_{n=1}^{N}\delta[\psi-\phi(\boldsymbol{r}^n,t)]. \tag{3.18}$$

Because the samples in the sample space ψ correspond to the ϕ values at different spatial locations ($\boldsymbol{r}^n$) within the subfilter volume in one flow realization, Eq. 3.18 is different from the discrete representation of the PDF (Eq. 2.2). It is also different from the first discrete representation of the FDF (Eq. 3.4) in two aspects. One is that Eq. 3.18 is valid for any filter function, while Eq. 3.4 is valid only for the box filter. The other is that ϕ^n in Eq. 3.18 evolve according to a transport equation for $F_\phi(\psi;\boldsymbol{x},t)$, which involves filtered quantities, while ϕ^n in Eq. 3.4 evolve according to Eq. 3.6, which requires quantities resolved at the smallest scales of turbulence.

In variable density inhomogeneous flows, the filtered mass density function (FMDF) has been defined as (Jaberi *et al.* 1999)

$$\mathscr{F}(\psi;\boldsymbol{x},t)=\int_{-\infty}^{+\infty}\rho(\boldsymbol{r},t)\delta[\psi-\phi(\boldsymbol{r},t)]G(|\boldsymbol{x}-\boldsymbol{r}|)d\boldsymbol{r}. \tag{3.19}$$

If we consider in Eq. 3.19 all the scalars $\boldsymbol{\phi}$ that determine the value of density $\rho=\rho(\boldsymbol{\phi})$ (e.g., in a low Mach number flow), then Eq. 3.19 is equivalent to

$$\mathscr{F}(\boldsymbol{\psi};\boldsymbol{x},t)=\int_{-\infty}^{+\infty}\rho(\boldsymbol{\psi})\boldsymbol{\delta}[\boldsymbol{\psi}-\boldsymbol{\phi}(\boldsymbol{r},t)]G(|\boldsymbol{x}-\boldsymbol{r}|)d\boldsymbol{r}=\rho(\boldsymbol{\psi})F(\boldsymbol{\psi};\boldsymbol{x},t), \tag{3.20}$$

where $\boldsymbol{\delta}[\boldsymbol{\psi}-\boldsymbol{\phi}(\boldsymbol{r},t)]$ represents the product of the 1-D delta functions $\delta[\psi_\alpha-\phi_\alpha(\boldsymbol{r},t)]$, and ψ_α is a component of $\boldsymbol{\psi}$. The reason for this equivalence is that multiplying a variable Q by either Eq. 3.19 or Eq. 3.20 and then integrating over ψ will give the same result as $\overline{\rho Q}$. It can be easily verified that FMDF satisfies the realizability, consistency, and normalization conditions as discussed in Pope (1985).

It is then desirable to have a discrete representation of the FMDF. Let M represent the total mass of fluid within a physical domain and this mass is equally distributed among N_t notational particles such that each particle has mass $\triangle m=M/N_t$. The nth particle has composition ϕ^n and position $\boldsymbol{r}^n$. With N_t and $\triangle m$ to be determined, the discrete

FMDF at time t is defined as

$$\mathscr{F}_N(\psi, \boldsymbol{x}; t) \equiv \triangle m \sum_{n=1}^{N(\boldsymbol{x},t)} \delta[\psi - \phi(\boldsymbol{r}^n, t)], \tag{3.21}$$

where $N(\boldsymbol{x})$ is the number of particles in the subfilter volume centered at position $\boldsymbol{x}$, and

$$N_t(t) = \int_{-\infty}^{+\infty} N(\boldsymbol{x}, t) d\boldsymbol{x}. \tag{3.22}$$

Not considered here are delta functions in physical space $\delta(\boldsymbol{X}^n - \boldsymbol{x})$, which is the norm in a Lagrangian PDF method; instead the number of particles N is specified as a function of $\boldsymbol{x}$. This reflects the nature of the filtering operation. Now, the properties of the delta functions in sample space and the specification of $N(\boldsymbol{x})$ are restricted by the requirement that the local expectation of $\mathscr{F}_N$ is the FMDF:

$$\overline{\mathscr{F}_N} = \mathscr{F}(\psi; \boldsymbol{x}, t). \tag{3.23}$$

Substituting Eq. 3.21 into Eq. 3.23 gives

$$\frac{M}{N_t} N(\boldsymbol{x}) \overline{\delta[\psi - \phi(\boldsymbol{r}^n, t)]} = \mathscr{F}(\psi; \boldsymbol{x}, t), \tag{3.24}$$

and a subsequent integration over ψ leads to

$$N(\boldsymbol{x}, t)/N_t(t) = \overline{\rho(\boldsymbol{x}, t)}/M. \tag{3.25}$$

Thus the number of particles within the subfilter volume centered at $\boldsymbol{x}$ is proportional to the filtered fluid density at $\boldsymbol{x}$. In addition, rewriting Eq. 3.24 as (with the substitution of Eq. 3.25 and Eq. 3.20)

$$\overline{\delta[\psi - \phi(\boldsymbol{r}^n, t)]} = \mathscr{F}(\psi; \boldsymbol{x}, t)/\overline{\rho} = \rho(\boldsymbol{\psi}) F(\boldsymbol{\psi}; \boldsymbol{x}, t)/\overline{\rho} = \tilde{F}(\boldsymbol{\psi}; \boldsymbol{x}, t) \tag{3.26}$$

shows that the FDF of notational particle properties centered at a given location $\boldsymbol{x}$ is equal to the density-weighted FDF at that location. Therefore, Eq. 3.25 and Eq. 3.26 determine the properties of $N(\boldsymbol{x})$ and the delta functions in Eq. 3.21 for the definition of a discrete FMDF.

4. Stochastic particle system for FDF transport

Due to the usually high dimensionality of FMDF, a Lagrangian particle method (Pope 1985) is typically employed to solve the transport FMDF equation. In Lagrangian PDF methods (Pope 1994), stochastic models/particles are constructed to simulate the evolution of fluid particle properties and to determine both Lagrangian and Eulerian PDFs. A key foundation of these methods is that the Lagrangian PDF is the transition density for the turbulent flow, which determines the transition of the Eulerian PDF from time t_0 to time t (Pope 1994). And a key component in these methods is establishing the correspondence between the stochastic particles and fluid particles such that the PDF represented by the stochastic particles evolves in the same way as the PDF of fluid particles (Pope 1985, 1994).

In the application of Lagrangian particle methods to transport FDF solutions, it seems impossible to define a Lagrangian FDF since a Lagrangian particle represents a single spatial point, while FDF involves a volume of space. However, the two discrete representations presented above clarify the issue.

If the first discrete representation (Eq. 3.3) is to be used, it is then unnecessary to define a Lagrangian FDF: it is straightforward to calculate the Eulerian FDF from fluid particles by simply using the definition of the FDF, which has built in the relationship between the FDF and fluid particles from one snapshot of the flow field. This implies that the solution to the Eulerian FDF transport equation is the same as the FDF evolved by fluid particles. The task of modeling is then to use the principle of stochastically equivalent systems (Pope 1985) and devise a stochastic process such that the Lagrangian PDF of the stochastic particles evolves in the same way as the delta function governed by Eq. 3.6. Although the Lagrangian PDF of the stochastic particles describe fluctuations over many flow realizations, on one flow realization the particles correspond to the delta functions that discretize the Lagrangian PDF and satisfy Eq. 3.6. Therefore, the Eulerian FDF can be approximated by the stochastic particles through Eq. 3.3.

If the second discrete representation (Eq. 3.18) is to be used, it is necessary to establish the relation between Eulerian FDF and Lagrangian particles from the perspective of PDF interpretation. The issue is that FDF/FPDF describes fluctuations on one flow realization, while Lagrangian PDF of particles describes fluctuations over many flow realizations. However, the Eulerian PDF derived from the particles (using the transition density property of Lagrangian PDF) can still correspond to the Eulerian FDF, which means that Eulerian PDF from the particles has the same functional form as the FDF, which is the subfilter PDF. It is essential though to realize that the delta functions for the discrete Eulerian PDF from particles (similar to Eq. 3.21), which are supposed to represent different flow realizations, now correspond to the delta functions for the discrete FDF (Eq. 3.21), which represent the samples in a subfilter volume on one flow realization. The task of modeling is then to use again the principle of stochastically equivalent systems (Pope 1985) and devise a stochastic process such that the Eulerian PDF derived from the stochastic particles evolves in the same way as the FDF governed by the FDF transport equation. The derivation of Eulerian PDF from stochastic/fluid particles has been described in detail by Pope (1985).

An example of the correspondence between FMDF and stochastic particles can be illustrated as follows. First, the transport equation for Eulerian FMDF based on Eq. 3.5 can be derived by multiplying Eq. 3.6 by the FDF $F(\boldsymbol{\phi};\boldsymbol{x},t)$ followed by integration over the sample space $\boldsymbol{\phi}$, which gives

$$\frac{\partial \rho(\boldsymbol{\psi})F_{\boldsymbol{\phi}}}{\partial t}+\frac{\partial\, \overline{u_i|\boldsymbol{\psi}}\,\rho(\boldsymbol{\psi})F_{\boldsymbol{\phi}}}{\partial x_i}=\frac{\partial}{\partial \psi_\alpha}\left[\overline{\frac{\partial J_i^\alpha}{\partial x_i}\bigg|\boldsymbol{\psi}}\,F_{\boldsymbol{\phi}}\right]-\frac{\partial}{\partial\psi_\alpha}\left[S_\alpha(\boldsymbol{\psi})\rho(\boldsymbol{\psi})F_{\boldsymbol{\phi}}\right]. \tag{4.1}$$

Then, substituting the definition of FMDF (Eq. 3.20) leads to

$$\frac{\partial \mathscr{F}_{\boldsymbol{\phi}}}{\partial t}+\frac{\partial\, \overline{u_i|\boldsymbol{\psi}}\,\mathscr{F}_{\boldsymbol{\phi}}}{\partial x_i}=\frac{\partial}{\partial \psi_\alpha}\left[\overline{\frac{1}{\rho}\frac{\partial J_i^\alpha}{\partial x_i}\bigg|\boldsymbol{\psi}}\,\mathscr{F}_{\boldsymbol{\phi}}\right]-\frac{\partial}{\partial\psi_\alpha}\left[S_\alpha(\boldsymbol{\psi})\mathscr{F}_{\boldsymbol{\phi}}\right]. \tag{4.2}$$

This equation is similar to Eq. 22 derived by Jaberi *et al.* (1999) using the filtering operation instead.

Next we wish to construct a system of stochastic particles in which the Eulerian mass density function (MDF, the product of density and PDF (Pope 1985)) calculated from the stochastic particles evolves in the same way as the solution to Eq. 4.2. Each particle possesses the properties of mass, position, velocity, and composition, denoted by $\triangle m^*$,

$\boldsymbol{x}^*(t)$, $u_j^*(t)$, and $\boldsymbol{\phi}^*(t)$, respectively. The MDF is approximated by

$$\mathscr{F}_{\boldsymbol{\phi}N}^*(\psi, \boldsymbol{x}; t) \equiv \triangle m^* \sum_{n=1}^{N(\boldsymbol{x},t)} \delta[\psi - \phi^*(\boldsymbol{r}_n^*, t)]. \tag{4.3}$$

The particle position and composition, respectively, evolve by

$$\frac{\mathrm{d}\boldsymbol{x}_j^*}{\mathrm{d}t} = u_j^*, \tag{4.4}$$

$$\frac{\mathrm{d}\phi_\alpha^*}{\mathrm{d}t} = \Theta_\alpha^* + S_\alpha(\boldsymbol{\psi}), \tag{4.5}$$

where Θ_α^* represents the molecular diffusion/mixing that need to be modeled. The corresponding evolution equation for the MDF $\mathscr{F}_{\boldsymbol{\phi}}^*$ is written as

$$\frac{\partial \mathscr{F}_{\boldsymbol{\phi}}^*}{\partial t} + \frac{\partial\, u_j^*\, \mathscr{F}_{\boldsymbol{\phi}}^*}{\partial x_i} = -\frac{\partial}{\partial \psi_\alpha}\left[\overline{\Theta_\alpha^* |\, \boldsymbol{\psi}}\, \mathscr{F}_{\boldsymbol{\phi}}\right] - \frac{\partial}{\partial \psi_\alpha}\left[S_\alpha(\boldsymbol{\psi}) \mathscr{F}_{\boldsymbol{\phi}}^*\right]. \tag{4.6}$$

In order for the particle process (Eq. 4.4 and 4.5) to model the transport equation for FMDF, Eq. 4.6 should be the same as Eq. 4.2. This determines that the particle velocity and mixing in Eq. 4.4 and 4.5 correspond, respectively, to the conditional filtered velocity and diffusion term in Eq. 4.2, which require modeling.

5. Implications for the mixing models

Because of the nature of discrete FDF (Eqs. 3.3, 3.18, and 4.3), particles in the sample space ψ correspond to particles in physical space at one instance of time, and they are close to each other in the subfilter volume. A mixing model in the FDF method will need to take advantage of this fact and more physics-based mixing models can be constructed. For example, in a particle-interaction type of model, a FDF particle may interact only with its surrounding particles and the extent of the interaction may depend on the distance between the interacting particles and the product of mixing time and diffusion coefficient. A mixing model may be designed as follows: suppose that in a particle implementation, particle i is surrounded by n_d particles that are immediately adjacent to particle i and may come from neighboring subfilter volumes, the mixing model may be written as

$$\phi^{*(i)}(t + \delta t) = \phi^{*(i)}(t) + \sum_{j=1}^{n_d} \frac{\phi^{*(j)}(t) - \phi^{*(i)}(t)}{r_{ij}} \frac{D_\phi \tau_\phi}{r_{ij}}, \tag{5.1}$$

where r_{ij} is the physical distance between particles i and j and D_ϕ is the molecular diffusivity. The first r_{ij} is used to show the influence of the concentration gradient between the particles and the second one is used to characterize the volume-area ratio for the mixing mass transfer. Since the local concentration gradient has been taken into account in the formulation, the mixing time τ_ϕ may simply be the physical time step in the LES simulation; this consequently avoids the time-scale estimations that are based on scalar dissipation rate, which requires modeling. For consistency, particle i must be included when the mixing model is applied to particle j. This model is deterministic, but the number of interacting particles n_d and the distance between particles r_{ij} vary stochastically with time. Note that the molecular diffusivity D_ϕ can be different for different scalars and this may simplify the treatment of differential diffusion.

In the LES/FDF approach for turbulent combustion, the modeling of molecular mixing is more important than that in the PDF method because the dependent chemical reaction rates affects the scalar fields and evolution instantaneously. Physics-based mixing models may become critical for the success of transported FDF methods. The kinetic theory of gases will be helpful in the design of a physics-based FDF mixing model since the FDF mixing represents the diffusion process within a subfilter volume at the small scales of turbulence. In addition, since the FDF mixing is instantaneous, DNS data will become very important, or may be the only resource, for the testing of a mixing model.

6. Conclusions

In an effort to resolve some of the issues in the development of the transported FDF methods for LES of turbulent combustion, two discrete representations of the FDF are presented and discussed. The first one is closely related to the definition of the FDF and is obtained from the numerical integration of the FDF. With this representation, a transport equation for the delta functions that approximate the FDF can be derived; it is straightforward to use the principle of stochastically equivalent systems and devise a stochastic particles system to solve the transport equation. Because of the irregularity within the subfilter volume, a large number of particles is required to increase the accuracy of the numerical integration of the FDF.

The second discrete representation is based on the fact that the FDF is the subfilter PDF, which is constructed from one flow realization and is, therefore, different from the PDF in the RANS context that is based on many flow realizations. This nature of FDF as the instantaneous subfilter PDF is discussed conceptually and mathematically. Based on this PDF view of FDF, the FDF can be discretized similarly to the RANS PDF and conditional filtered values can be defined and interpreted as conditional averaged values. Following the same line of thinking, a method to calculate FDF from the DNS data using different filter functions is proposed. For variable density inhomogeneous flows, an original discrete representation of FMDF is proposed and the modeling principle for the FMDF transport equation is discussed.

In both discrete representations, the delta functions correspond to particles in the physical space within the subfilter volume at one instance of time. A more physics-based mixing model is proposed to take into account this characteristic. The advantages of this more physics-based model include that mixing time scale estimations based on scalar dissipation rate can be avoided and that differential diffusion can be easily treated. Because of the nature of the FDF mixing, it is noted that the kinetic theory of gases will be useful in the design of FDF mixing models and DNS data will become very important in the testing of the mixing models.

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