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Density Weighted FDF Equations for Simulations of Turbulent Reacting Flows

Tsan-Hsing Shih
Ohio Aerospace Institute, Brook Park, Ohio

Nan-Suey Liu
Glenn Research Center, Cleveland, Ohio

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Tsan-Hsing Shih
Ohio Aerospace Institute, Brook Park, Ohio

Nan-Suey Liu
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National Aeronautics and
Space Administration

Glenn Research Center
Cleveland, Ohio 44135

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Tsan-Hsing Shih
Ohio Aerospace Institute
Brook Park, Ohio 44142

Nan-Suey Liu
National Aeronautics and Space Administration
Glenn Research Center
Cleveland, Ohio 44135

Abstract

In this report, we briefly revisit the formulation of density weighted filtered density function (DW-FDF) for large eddy simulation (LES) of turbulent reacting flows, which was proposed by Jaberi et al. (Ref. 1). At first, we proceed the traditional derivation of the DW-FDF equations by using the fine grained probability density function (FG-PDF), then we explore another way of constructing the DW-FDF equations by starting directly from the compressible Navier-Stokes equations. We observe that the terms which are unclosed in the traditional DW-FDF equations are now closed in the newly constructed DW-FDF equations. This significant difference and its practical impact on the computational simulations may deserve further studies.

1.0 Introduction

The concept of filtered density function (FDF) method (Ref. 2) was extended to the compressible turbulent reacting flow by introducing a filtered mass density function (FMDF) (Ref. 1), which is a density weighted FDF and is referred as DW-FDF in this report. The work was considered as the extension of the probability density function (PDF) method (Pope (Ref. 3)) to the LES simulation with the advantage of its direct simulation of turbulence-chemistry interaction without modeling.

This report follows our previous work on the conservational PDF equations (Shih and Liu (Ref. 4)) to explore different ways of constructing the DW-FDF equations for simulations of filtered turbulent reacting flows. It will be shown that there are significant differences between the FMDF equations and the newly proposed DW-FDF equations, with the latter requiring much less empirical modeling.

In Section 2.0, we review the definition of DW-FDF starting from a delta function of a turbulent random variable, which is called in the literature as the fine grained probability density function (FG-PDF) f'. The definition of a filtered turbulent variable used in LES is also briefly reviewed. Then we explore the relationship between the DW-FDF and the filtered turbulent variable. This relationship suggests the concept of "DW-FDF mean", $\langle\ \rangle_L$ which is the analogy to the statistical mean, $\langle\ \rangle$ in the PDF theory. A few properties of the DW-FDF mean are explored, and they are found to be useful in constructing the transport equations for the DW-FDF.

In Section 3.0, we first formulate a compressible transport equation for FG-PDF, and then apply a stationary or homogeneous filtering on it to construct the equations that we refer as the traditional DW-FDF equations, which are consistent with the FMDF equations introduced by Jaberi et al. (Ref. 1).

In Section 4.0, we adopt a similar methodology described in Reference 4 to construct the DW-FDF equations by directly starting from the filtered compressible Navier-Stokes equations. The resulted equations are significantly different from the traditional FMDF equations. For example, the unclosed terms appearing on the right hand side of FMDF equations are now closed in the newly constructed DW-FDF equations.

It is noted here that the quantity DW-FDF (or FMDF) is fundamentally different from the quantity PDF, namely, DW-FDF is a random quantity; but PDF is a deterministic quantity. The "DW-FDF mean" defines a density-weighted filtered turbulent random variable; but the "PDF mean" defines a turbulent mean variable. The DW-FDF, unlike PDF, does not represent a probability density of a random variable; it is only a density-weighted filtered FG-PDF and is still a random variable. These fundamental differences between DW-FDF and PDF may require a further investigation on their respective solution procedures based on the stochastic differential equation methods.

2.0 Density Weighted Filtered Density Function (DW-FDF) and Filtered Turbulent Variables

In this section, we will first review the basic properties of FG-PDF and its density-weighted filtered quantity, DW-FDF, then explore the relationship between DW-FDF and filtered turbulent variable. This provides the basis for further establishing the transport equations of DW-FDF.

2.1 Fine Grained Probability Density Function (FG-PDF) $f'_U\left(\boldsymbol{V}\,;\boldsymbol{x},t\right)$, $f'_\Phi\left(\boldsymbol{\psi}\,;\boldsymbol{x},t\right)$

The FG-PDF for turbulent velocity and scalars (e.g., species mass fraction, internal energy) are defined as follows (Pope (Ref. 3)),

$$f'_U(\boldsymbol{V};\boldsymbol{x},t) \equiv \delta\left(\boldsymbol{U}(\boldsymbol{x},t)-\boldsymbol{V}\right) \equiv \prod_{i=1}^{3} \delta\left(U_i(\boldsymbol{x},t)-V_i\right) \tag{1}$$

$$f'_\Phi(\boldsymbol{\psi};\boldsymbol{x},t) \equiv \delta\left(\boldsymbol{\Phi}(\boldsymbol{x},t)-\boldsymbol{\psi}\right) \equiv \prod_{i=1}^{N+1} \delta\left(\Phi_i(\boldsymbol{x},t)-\psi_i\right) \tag{2}$$

where δ denotes the delta function, $\boldsymbol{U}(\boldsymbol{x},t)$ is the turbulent velocity vector (U_1, U_2, U_3), $\boldsymbol{\Phi}(\boldsymbol{x},t)$ is the turbulent scalar array ($\Phi_1, \Phi_2,\cdots, \Phi_N, \Phi_{N+1}$), for example, N species mass fractions and one internal energy $\Phi_{N+1} = e$, the $\boldsymbol{x},t$ denote the physical space variable (x_1, x_2, x_3) and the time t, $\boldsymbol{V} \equiv (V_1, V_2, V_3)$ and $\boldsymbol{\psi} \equiv (\psi_1, \psi_2,\cdots, \psi_N, \psi_{N+1})$ are the sample space variables for $\boldsymbol{U}(\boldsymbol{x},t)$ and $\boldsymbol{\Phi}(\boldsymbol{x},t)$, respectively. The FG-PDF has the following properties that will be used in this study:

i. The Unity Integral of FG-PDF

$$\int_{-\infty}^{+\infty} f'_U\left(\boldsymbol{V};\boldsymbol{x},t\right)d\boldsymbol{V} = 1, \quad \int_{-\infty}^{+\infty} f'_\Phi\left(\boldsymbol{\psi};\boldsymbol{x},t\right)d\boldsymbol{\psi} = 1 \tag{3}$$

Note that $(-\infty, +\infty)$ represents the whole domain of sample space, for the species mass fractions it really means (0,1).

ii. The Differential Chain

$$\frac{\partial f'_U}{\partial t} = \frac{\partial f'_U}{\partial U_i}\frac{\partial U_i}{\partial t} = -\frac{\partial f'_U}{\partial V_i}\frac{\partial U_i}{\partial t} = -\frac{\partial}{\partial V_i}\left(f'_U\frac{\partial U_i}{\partial t}\right) \tag{4}$$

$$\frac{\partial f'_U}{\partial x_j} = \frac{\partial f'_U}{\partial U_i}\frac{\partial U_i}{\partial x_j} = -\frac{\partial f'_U}{\partial V_i}\frac{\partial U_i}{\partial x_j} = -\frac{\partial}{\partial V_i}\left(f'_U\frac{\partial U_i}{\partial x_j}\right) \tag{5}$$

Note that the summation convention on the same index, e.g., "i" is implied. Therefore, we have

$$\frac{\partial f_U'}{\partial t}+U_j\frac{\partial f_U'}{\partial x_j}=-\frac{\partial}{\partial V_i}\left[f_U'\left(\frac{\partial U_i}{\partial t}+U_j\frac{\partial U_i}{\partial x_j}\right)\right],\quad \text{(for incompressible flow)}\quad i,j=1,2,3 \tag{6}$$

and

$$\frac{\partial \rho f_U'}{\partial t}+\frac{\partial \rho U_j f_U'}{\partial x_j}=-\frac{\partial}{\partial V_i}\left[f_U'\left(\frac{\partial \rho U_i}{\partial t}+\frac{\partial \rho U_i U_j}{\partial x_j}\right)\right],\quad \text{(for compressible flow)}\quad i,j=1,2,3 \tag{7}$$

Note that the continuity equation of compressible flow has been applied here. Similarly,

$$\frac{\partial f_\Phi'}{\partial t}=\frac{\partial f_\Phi'}{\partial \Phi_i}\frac{\partial \Phi_i}{\partial t}=-\frac{\partial f_\Phi'}{\partial \psi_i}\frac{\partial \Phi_i}{\partial t}=-\frac{\partial}{\partial \psi_i}\left(f_\Phi'\frac{\partial \Phi_i}{\partial t}\right) \tag{8}$$

$$\frac{\partial f_\Phi'}{\partial x_j}=\frac{\partial f_\Phi'}{\partial \Phi_i}\frac{\partial \Phi_i}{\partial x_j}=-\frac{\partial f_\Phi'}{\partial \psi_i}\frac{\partial \Phi_i}{\partial x_j}=-\frac{\partial}{\partial \psi_i}\left(f_\Phi'\frac{\partial \Phi_i}{\partial x_j}\right) \tag{9}$$

and

$$\frac{\partial f_\Phi'}{\partial t}+U_j\frac{\partial f_\Phi'}{\partial x_j}=-\frac{\partial}{\partial \psi_i}\left[f_\Phi'\left(\frac{\partial \Phi_i}{\partial t}+U_j\frac{\partial \Phi_i}{\partial x_j}\right)\right],\quad \text{(for incompressible flow)}\begin{cases}i=1,2,\cdots,N+1\\ j=1,2,3\end{cases} \tag{10}$$

$$\frac{\partial \rho f_\Phi'}{\partial t}+\frac{\partial \rho U_j f_\Phi'}{\partial x_j}=-\frac{\partial}{\partial \psi_i}\left[f_\Phi'\left(\frac{\partial \rho \Phi_i}{\partial t}+\frac{\partial \rho \Phi_i U_j}{\partial x_j}\right)\right],\text{(for compressible flow)}\begin{cases}i=1,2,\cdots,N+1\\ j=1,2,3\end{cases} \tag{11}$$

iii. The Sifting Property

$$\boldsymbol{U}(\boldsymbol{x},t)\,f_U'(\boldsymbol{V};\boldsymbol{x},t)\equiv\boldsymbol{U}(\boldsymbol{x},t)\delta\big(\boldsymbol{U}(\boldsymbol{x},t)-\boldsymbol{V}\big)=\boldsymbol{V}\delta\big(\boldsymbol{U}(\boldsymbol{x},t)-\boldsymbol{V}\big)=\boldsymbol{V}\,f_U'(\boldsymbol{V};\boldsymbol{x},t) \tag{12}$$

$$\boldsymbol{\Phi}(\boldsymbol{x},t)f_\Phi'(\boldsymbol{\psi};\boldsymbol{x},t)=\boldsymbol{\psi}\,f_\Phi'(\boldsymbol{\psi};\boldsymbol{x},t) \tag{13}$$

More generally,

$$\begin{aligned}Q\big(\boldsymbol{U}(\boldsymbol{x},t)\big)f_U'(\boldsymbol{V};\boldsymbol{x},t)&=Q(\boldsymbol{V})\,f_U'(\boldsymbol{V};\boldsymbol{x},t)\\ Q\big(\boldsymbol{\Phi}(\boldsymbol{x},t)\big)f_\Phi'(\boldsymbol{\psi};\boldsymbol{x},t)&=Q(\boldsymbol{\psi})\,f_\Phi'(\boldsymbol{\psi};\boldsymbol{x},t)\end{aligned} \tag{14}$$

where $Q(\ )$ denotes a general (but not the time or space differential) function form.

iv. The Statistical Mean of FG-PDF

Equations (1) and (2) indicate that FG-PDF is a random quantity, because it is the delta function of the random variable $\boldsymbol{U}(\boldsymbol{x},t)$ or $\boldsymbol{\Phi}(\boldsymbol{x},t)$. The basic probability theory says that a random variable and its (non-differential) function share the same probability density. Therefore, the probability density function PDF of the random variable FG-PDF is $f_U\,(\boldsymbol{V};\boldsymbol{x},t)$ or $f_\Phi(\boldsymbol{\psi};\boldsymbol{x},t)$, which is the PDF of turbulent velocity

$\boldsymbol{U}(\boldsymbol{x},t)$ or scalars $\boldsymbol{\Phi}(\boldsymbol{x},t)$, respectively. It is easy to verify that the statistical mean of FG-PDF is the corresponding PDF (Pope (Ref. 3)):

$$\left\langle f'_U(\boldsymbol{V};\boldsymbol{x},t)\right\rangle = \left\langle \delta\left(\boldsymbol{U}(\boldsymbol{x},t)-\boldsymbol{V}\right)\right\rangle \equiv \int_{-\infty}^{+\infty} \delta\left(\boldsymbol{V}'-\boldsymbol{V}\right) f_U(\boldsymbol{V}';\boldsymbol{x},t)\, d\boldsymbol{V}' = f_U(\boldsymbol{V};\boldsymbol{x},t) \tag{15}$$

Similarly,

$$\left\langle f'_\Phi(\boldsymbol{\psi};\boldsymbol{x},t)\right\rangle = f_\Phi(\boldsymbol{\psi};\boldsymbol{x},t) \tag{16}$$

The FG-PDF is a useful quantity for mathematical derivations. It is interesting to examine the following expressions:

$$\int \boldsymbol{V}\, f'_U(\boldsymbol{V};\boldsymbol{x},t)\, d\boldsymbol{V} \equiv \left\langle \boldsymbol{U}(\boldsymbol{x},t)\right\rangle_{FG} = \boldsymbol{U}(\boldsymbol{x},t) \tag{17}$$

$$\int \boldsymbol{\psi}\, f'_\Phi(\boldsymbol{\psi};\boldsymbol{x},t)\, d\boldsymbol{\psi} \equiv \left\langle \boldsymbol{\Phi}(\boldsymbol{x},t)\right\rangle_{FG} = \boldsymbol{\Phi}(\boldsymbol{x},t) \tag{18}$$

which indicate that the "FG-PDF mean" defines the original random variable itself. More generally,

$$\begin{aligned}
&\int Q(\boldsymbol{V})\, f'_U(\boldsymbol{V};\boldsymbol{x},t)\, d\boldsymbol{V} \equiv \left\langle Q\left(\boldsymbol{U}(\boldsymbol{x},t)\right)\right\rangle_{FG} = Q\left(\boldsymbol{U}(\boldsymbol{x},t)\right) \\
&\int Q(\boldsymbol{\psi})\, f'_\Phi(\boldsymbol{\psi};\boldsymbol{x},t)\, d\boldsymbol{\psi} \equiv \left\langle Q\left(\boldsymbol{\Phi}(\boldsymbol{x},t)\right)\right\rangle_{FG} = Q\left(\boldsymbol{\Phi}(\boldsymbol{x},t)\right)
\end{aligned} \tag{19}$$

2.2 Filtered Turbulent Variables and DW-FDF $F_U\left(\boldsymbol{V};\boldsymbol{x},t\right)$, $f_\Phi\left(\boldsymbol{\psi};\boldsymbol{x},t\right)$

First we review the definition of filtered turbulent variables conventionally used in the turbulent simulation and the definition of DW-FDF, and then we explore the relationship between the DW-FDF and the filtered turbulent variables.

2.2.1 Filtered Turbulent Variables

In the conventional simulation of compressible reacting flows, we often deal with two types of filtered turbulent variables: one with the density weighting, the other without the density weighting. The filtered turbulent variable without the density weighting is denoted by $\bar{\phi}(\boldsymbol{x},t)$ and is defined as

$$\bar{\phi}(\boldsymbol{x},t) = \int_{-\infty}^{+\infty} \phi(\boldsymbol{x},t')\, G(t-t')\, dt' \tag{20}$$

where ϕ is the unfiltered turbulent variable, e.g., velocity components U_i, density ρ, pressure P, species mass fraction Φ_i and internal energy $e = \sum_{m=1}^{N} \Phi_m e_m$. The integration is over the entire time domain $-\infty < t' < +\infty$. $G(t-t')$ is the time filter with a constant filter width Δ_T and satisfies the following condition and asymptotic property:

$$\int_{-\infty}^{+\infty} G(t-t')\, dt' = 1 \tag{21}$$

$$\int_{-\infty}^{+\infty} \phi(\boldsymbol{x},t')\, G(t-t')\, dt' = \phi(\boldsymbol{x},t), \quad \text{as } \Delta_T \to 0 \tag{22}$$

The density-weighted filtered turbulent variable is denoted by $\tilde{\phi}(\boldsymbol{x},t)$ and defined as

$$\tilde{\phi}(\boldsymbol{x},t) = \frac{\overline{\rho\phi}}{\overline{\rho}} \tag{23}$$

It is noted here that these filtered variables $\overline{\phi}(\boldsymbol{x},t)$, $\tilde{\phi}(\boldsymbol{x},t)$ represent the large scale turbulent variables (Shih and Liu (Refs. 5 and 6)), and they are still random but contain relatively low frequency part of the turbulent motion when comparing with the unfiltered turbulent variable $\phi(\boldsymbol{x},\boldsymbol{t})$.

2.2.2 Definition of DW-FDF

Jaberi et al. (Ref. 1) introduced the density-weighted space filter operation $\rho(\boldsymbol{x}',t)\mathrm{G}(\boldsymbol{x}-\boldsymbol{x}')$ on the FG-PDF $f'_U(\boldsymbol{V};\boldsymbol{x},t)$, $f'_\Phi(\psi;\boldsymbol{x},t)$ and referred to them as the filtered mass density function FMDF. However, we prefer a more intuitive name related to the existing FDF methodology (Colluci et al. (Ref. 2)), and refer them as the density weighted FDF (DW-FDF). With the density-weighted time filter $\rho(\boldsymbol{x},t')\mathrm{G}(t-t')$ we define the following marginal DW-FDF as

$$\begin{aligned}
F_U(\boldsymbol{V};\boldsymbol{x},t) &\equiv \int_{-\infty}^{+\infty} \rho\left(\boldsymbol{x},t'\right) f'_U(\boldsymbol{V};\boldsymbol{x},t')\, G(t-t')\, dt' \\
&= \int_{-\infty}^{+\infty} \rho\left(\boldsymbol{x},t'\right) \delta\left(\boldsymbol{U}\left(\boldsymbol{x},t'\right)-\boldsymbol{V}\right) G(t-t')\, dt' \\
F_\Phi(\psi;\boldsymbol{x},t) &\equiv \int_{-\infty}^{+\infty} \rho\left(\boldsymbol{x},t'\right) f'_\Phi(\psi;\boldsymbol{x},t')\, G(t-t')\, dt' \\
&= \int_{-\infty}^{+\infty} \rho\left(\boldsymbol{x},t'\right) \delta\left(\boldsymbol{\Phi}\left(\boldsymbol{x},t'\right)-\psi\right) G(t-t')\, dt'
\end{aligned} \tag{24}$$

Obviously, DW-FDF, i.e., $F_U(\boldsymbol{V};\boldsymbol{x},t)$ or $F_\Phi(\psi;\boldsymbol{x},t)$, is still a random quantity. It satisfies the following "normalization" property:

$$\begin{aligned}
\int_{-\infty}^{\infty} F_U(\boldsymbol{V};\boldsymbol{x},t)\, d\boldsymbol{V} &= \int_{-\infty}^{\infty} \int_{-\infty}^{+\infty} \rho\left(\boldsymbol{x},t'\right) f'_U(\boldsymbol{V};\boldsymbol{x},t')\, G(t-t')\, dt'\, d\boldsymbol{V} = \int_{-\infty}^{+\infty} \rho\left(\boldsymbol{x},t'\right) G(t-t')\, dt' = \overline{\rho} \\
\int_{-\infty}^{\infty} F_\Phi(\psi;\boldsymbol{x},t)\, d\boldsymbol{\psi} &= \int_{-\infty}^{\infty} \int_{-\infty}^{+\infty} \rho\left(\boldsymbol{x},t'\right) f'_\Phi(\psi;\boldsymbol{x},t')\, G(t-t')\, dt'\, d\psi = \int_{-\infty}^{+\infty} \rho\left(\boldsymbol{x},t'\right) G(t-t')\, dt' = \overline{\rho}
\end{aligned} \tag{25}$$

With the definition of DW-FDF described in Equation (24), we can exactly deduce the filtered turbulent variables that are conventionally defined by Equations (20) and (23). For example,

$$\begin{aligned}
\int_{-\infty}^{+\infty} \boldsymbol{V} F_U(\boldsymbol{V};\boldsymbol{x},t)\, d\boldsymbol{V} &= \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \boldsymbol{V} \rho\left(\boldsymbol{x},t'\right) \delta\left(\boldsymbol{U}\left(\boldsymbol{x},t'\right)-\boldsymbol{V}\right) G(t-t')\, dt' d\boldsymbol{V} \\
&= \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \boldsymbol{U}\left(\boldsymbol{x},t'\right) \rho\left(\boldsymbol{x},t'\right) \delta\left(\boldsymbol{U}\left(\boldsymbol{x},t'\right)-\boldsymbol{V}\right) G(t-t')\, dt' d\boldsymbol{V} \\
&= \int_{-\infty}^{+\infty} \rho\left(\boldsymbol{x},t'\right) \boldsymbol{U}\left(\boldsymbol{x},t'\right) G(t-t')\, dt' = \overline{\rho \boldsymbol{U}} = \overline{\rho}\left(\boldsymbol{x},t\right) \tilde{\boldsymbol{U}}(\boldsymbol{x},t)
\end{aligned} \tag{26}$$

where the sifting property of FG-PDF has been used in the second line of (26). Similarly,

$$\int_{-\infty}^{+\infty} \boldsymbol{\psi}\, F_{\Phi}\left(\boldsymbol{\psi}\,;\,\boldsymbol{x},t\right) d\boldsymbol{\psi} = \overline{\rho\boldsymbol{\Phi}} = \overline{\rho}\left(\boldsymbol{x},t\right)\tilde{\boldsymbol{\Phi}}\left(\boldsymbol{x},t\right) \tag{27}$$

If we denote the left hand side of Equations (26) and (27) as the operation $\langle \boldsymbol{U}\rangle_L$ and $\langle \boldsymbol{\Phi}\rangle_L$, we may write Equations (26) and (27) as

$$\left\langle \boldsymbol{U}\right\rangle_L \equiv \int_{-\infty}^{+\infty} \boldsymbol{V}\, F_U(\boldsymbol{V}\,;\,\boldsymbol{x},t)\, d\boldsymbol{V} = \overline{\rho}\left(\boldsymbol{x},t\right)\tilde{\boldsymbol{U}}\left(\boldsymbol{x},t\right) \tag{28}$$

$$\left\langle \boldsymbol{\Phi}\right\rangle_L \equiv \int_{-\infty}^{+\infty} \boldsymbol{\psi}\, F_{\Phi}(\boldsymbol{\psi}\,;\,\boldsymbol{x},t)\, d\boldsymbol{\psi} = \overline{\rho}\left(\boldsymbol{x},t\right)\tilde{\boldsymbol{\Phi}}\left(\boldsymbol{x},t\right) \tag{29}$$

and for the function $Q(\boldsymbol{U}(\boldsymbol{x},t))$ or $W(\boldsymbol{\Phi}(\boldsymbol{x},t))$,

$$\begin{aligned} \left\langle Q\left(\boldsymbol{U}\right)\right\rangle_L &= \int_{-\infty}^{+\infty} Q(\boldsymbol{V})\, F_U(\boldsymbol{V}\,;\,\boldsymbol{x},t)\, d\boldsymbol{V} = \overline{\rho}\left(\boldsymbol{x},t\right)\tilde{Q}\left(\boldsymbol{U}(\boldsymbol{x},t)\right) \\ \left\langle W\left(\boldsymbol{\Phi}\right)\right\rangle_L &= \int_{-\infty}^{+\infty} W(\boldsymbol{\psi})\, F_{\Phi}(\boldsymbol{\psi}\,;\,\boldsymbol{x},t)\, d\boldsymbol{\psi} = \overline{\rho}\left(\boldsymbol{x},t\right)\tilde{W}\left(\boldsymbol{\Phi}(\boldsymbol{x},t)\right) \end{aligned} \tag{30}$$

Furthermore, we may consider the derivatives ∇P, $\nabla \boldsymbol{U}$, $\nabla \boldsymbol{\Phi}$ as the new random quantities and legitimately write

$$\left\langle \nabla P\right\rangle_L = \overline{\rho}\,\widetilde{\nabla P}\nabla P, \quad \left\langle \nabla \boldsymbol{U}\right\rangle_L = \overline{\rho}\,\widetilde{\nabla \boldsymbol{U}}, \quad \left\langle \nabla \boldsymbol{\Phi}\right\rangle_L = \overline{\rho}\,\widetilde{\nabla \boldsymbol{\Phi}} \tag{31}$$

However, the operation $\langle\ \rangle_L$ does not have the differential commute property, i.e.

$$\left\langle \nabla P\right\rangle_L \neq \nabla\left\langle P\right\rangle_L, \quad \left\langle \nabla \boldsymbol{U}\right\rangle_L \neq \nabla\left\langle \boldsymbol{U}\right\rangle_L, \quad \left\langle \nabla \boldsymbol{\Phi}\right\rangle_L \neq \nabla\left\langle \boldsymbol{\Phi}\right\rangle_L \tag{32}$$

because $\overline{\rho}\,\widetilde{\nabla P} \neq \nabla\left(\overline{\rho}\tilde{P}\right)$, $\overline{\rho}\,\widetilde{\nabla \boldsymbol{U}} \neq \nabla\left(\overline{\rho}\tilde{\boldsymbol{U}}\right)$, $\overline{\rho}\,\widetilde{\nabla \boldsymbol{\Phi}} \neq \nabla\left(\overline{\rho}\tilde{\boldsymbol{\Phi}}\right)$.

It can be verified that

$$\left\langle U_i U_j\right\rangle_L = \int_{-\infty}^{+\infty} V_i V_j\, F_U(\boldsymbol{V}\,;\,\boldsymbol{x},t)\, d\boldsymbol{V} = \overline{\rho}\left(\boldsymbol{x},t\right)\widetilde{U_i U_j}(\boldsymbol{x},t) \tag{33}$$

We can also write $\left\langle U_j \Phi_i\right\rangle_L$ for the joint variables as

$$\left\langle U_j \Phi_i\right\rangle_L = \int_{-\infty}^{+\infty} V_j\, \psi_i\, F_{U,\Phi}(\boldsymbol{V},\boldsymbol{\psi}\,;\,\boldsymbol{x},t)\, d\boldsymbol{V} d\boldsymbol{\psi} = \overline{\rho}\left(\boldsymbol{x},t\right)\widetilde{U_j \Phi_i}(\boldsymbol{x},t) \tag{34}$$

where, $F_{U,\Phi}(\boldsymbol{V},\boldsymbol{\psi};\,\boldsymbol{x},t)$ is the joint DW-FDF defined as

$$F_{U,\Phi}(\boldsymbol{V},\boldsymbol{\psi}\,;\,\boldsymbol{x},t) = \int_{-\infty}^{+\infty} \rho\left(\boldsymbol{x},t'\right)\delta\left(\boldsymbol{U}\left(\boldsymbol{x},t'\right)-\boldsymbol{V}\right)\delta\left(\boldsymbol{\Phi}\left(\boldsymbol{x},t'\right)-\boldsymbol{\psi}\right)G(t-t')\, dt' \tag{35}$$

which also satisfies the normalization property:

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} F_{U,\Phi}(\boldsymbol{V},\boldsymbol{\psi}\,;\,\boldsymbol{x},t)\, d\boldsymbol{V} d\boldsymbol{\psi} = \int_{-\infty}^{+\infty} \rho\left(\boldsymbol{x},t'\right)G(t-t')\, dt' = \overline{\rho} \tag{36}$$

2.2.3 DW-FDF Mean $\langle\ \rangle_L$

Analogous to $\int \boldsymbol{V} f_U(\boldsymbol{V};\boldsymbol{x},t)d\boldsymbol{V} = \langle \mathbf{U}(\boldsymbol{x},t)\rangle$, which defines the statistical mean of the random velocity by its PDF f_U, we may refer the operation $\langle\ \rangle_L$ as the "DW-FDF-mean", which defines the density weighted filtered turbulent variable, e.g., $\langle \boldsymbol{U}\rangle_L = \overline{\rho \boldsymbol{U}}$, $\langle U_j \Phi_i\rangle_L = \overline{\rho U_j \Phi_i}$ (see Eqs. (28) to (34)). From Equation (35), we may follow Pope (Ref. 3) to define a "conditional" DW-FDF on the condition $\boldsymbol{\Phi} = \boldsymbol{\psi}$ as

$$F_{U|\Phi}(\boldsymbol{V}|\,\boldsymbol{\psi};\boldsymbol{x},t) \equiv \frac{F_{U,\Phi}(\boldsymbol{V},\boldsymbol{\psi};\boldsymbol{x},t)}{F_{\Phi}(\boldsymbol{\psi};\boldsymbol{x},t)} \tag{37}$$

and the "conditional DW-FDF-mean" as

$$\begin{aligned}
\langle \boldsymbol{U}(\boldsymbol{x},t)|\,\boldsymbol{\psi}\rangle_L &\equiv \int_{-\infty}^{+\infty} \boldsymbol{V} F_{U|\Phi}(\boldsymbol{V}|\,\boldsymbol{\psi};\boldsymbol{x},t)\,d\boldsymbol{V} = \frac{1}{F_{\Phi}(\boldsymbol{\psi};\boldsymbol{x},t)}\int_{-\infty}^{+\infty} \boldsymbol{V} F_{U,\Phi}(\boldsymbol{V},\boldsymbol{\psi};\boldsymbol{x},t)\,d\boldsymbol{V} \\
&= \frac{1}{F_{\Phi}}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \boldsymbol{V}\rho(\boldsymbol{x},t')\delta\left(\boldsymbol{U}(\boldsymbol{x},t')-\boldsymbol{V}\right)\delta\left(\boldsymbol{\Phi}(\boldsymbol{x},t')-\boldsymbol{\psi}\right)G(t-t')\,dt'd\boldsymbol{V} \\
&= \frac{1}{F_{\Phi}}\int_{-\infty}^{+\infty} \rho(\boldsymbol{x},t')\boldsymbol{U}(\boldsymbol{x},t')\delta\left(\boldsymbol{\Phi}(\boldsymbol{x},t')-\boldsymbol{\psi}\right)G(t-t')\,dt'
\end{aligned} \tag{38}$$

Then we have

$$\int_{-\infty}^{+\infty} \rho(\boldsymbol{x},t')\boldsymbol{U}(\boldsymbol{x},t')f'_{\Phi}(\boldsymbol{\psi};\boldsymbol{x},t')G(t-t')\,dt' = \int_{-\infty}^{+\infty} \boldsymbol{V} F_{U,\Phi}(\boldsymbol{V},\boldsymbol{\psi};\boldsymbol{x},t)\,d\boldsymbol{V} = F_{\Phi}\cdot\langle \boldsymbol{U}(\boldsymbol{x},t)|\,\boldsymbol{\psi}\rangle_L \tag{39}$$

and

$$\begin{aligned}
\int_{-\infty}^{+\infty}\left(F_{\Phi}\cdot\langle \boldsymbol{U}(\boldsymbol{x},t)|\,\boldsymbol{\psi}\rangle_L\right)d\boldsymbol{\psi} &= \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \boldsymbol{V} F_{U,\Phi}(\boldsymbol{V},\boldsymbol{\psi};\boldsymbol{x},t)\,d\boldsymbol{V}d\boldsymbol{\psi} \\
&= \int_{-\infty}^{+\infty} \rho(\boldsymbol{x},t')\boldsymbol{U}(\boldsymbol{x},t')G(t-t')\,dt' \\
&= \overline{\rho}(\boldsymbol{x},t)\tilde{\boldsymbol{U}}(\boldsymbol{x},t)
\end{aligned} \tag{40}$$

Equation (39) can be extended to any other turbulent quantities, for example, ∇P, $\nabla \boldsymbol{U}$, $\nabla\boldsymbol{\Phi}$, $S_i(\boldsymbol{\Phi})$:

$$\begin{aligned}
&\int_{-\infty}^{+\infty} \rho(\boldsymbol{x},t')\nabla P(\boldsymbol{x},t')\,f'_U(\boldsymbol{V};\boldsymbol{x},t')\,G(t-t')\,dt' = F_U\cdot\langle \nabla P|\boldsymbol{V}\rangle_L \\
&\int_{-\infty}^{+\infty} \rho(\boldsymbol{x},t')\nabla \boldsymbol{U}(\boldsymbol{x},t')\,f'_U(\boldsymbol{V};\boldsymbol{x},t')\,G(t-t')\,dt' = F_U\cdot\langle \nabla \boldsymbol{U}|\boldsymbol{V}\rangle_L \\
&\int_{-\infty}^{+\infty} \rho(\boldsymbol{x},t')\nabla \boldsymbol{\Phi}(\boldsymbol{x},t')\,f'_{\Phi}(\boldsymbol{\psi};\boldsymbol{x},t')\,G(t-t')\,dt' = F_{\Phi}\cdot\langle \nabla \boldsymbol{\Phi}|\,\boldsymbol{\psi}\rangle_L \\
&\int_{-\infty}^{+\infty} \rho(\boldsymbol{x},t')S_i\left(\boldsymbol{\Phi}(\boldsymbol{x},t')\right)f'_{\Phi}(\boldsymbol{\psi};\boldsymbol{x},t')\,G(t-t')\,dt' = F_{\Phi}\cdot\langle S_i(\boldsymbol{\Phi})|\,\boldsymbol{\psi}\rangle_L = F_{\Phi}\cdot S_i(\boldsymbol{\psi})
\end{aligned} \tag{41}$$

where ∇P, $\nabla \boldsymbol{U}$, $\nabla\boldsymbol{\Phi}$, are viewed as the random variables in addition to P, $\boldsymbol{U}$, $\boldsymbol{\Phi}$.

3.0 Traditional DW-FDF Equations for $F_U(\boldsymbol{V}\,;\boldsymbol{x},t), F_\Phi(\boldsymbol{\psi}\,;\boldsymbol{x},t)$

In this section, we briefly review the traditional way of deriving DW-FDF equations starting from the equation of FG-PDF. The "exact" but not closed DW-FDF equations are derived, which are consistent with the traditional FMDF equations introduced by Jaberi et al. (Ref. 1).

3.1 Traditional DW-FDF Equation for $F_U(\boldsymbol{V}\,;\boldsymbol{x},t)$

The transport equation for the fine grained PDF with the variable density $\rho(\boldsymbol{x},t)$ can be written as (see Equation (7)):

$$\frac{\partial \rho f_U'}{\partial t}+\frac{\partial \rho U_j f_U'}{\partial x_j}=-\frac{\partial}{\partial V_i}\left\{f_U'\left(-\frac{\partial P}{\partial x_i}+\frac{\partial}{\partial x_j}\left(2\mu S_{ij}-\frac{2}{3}\mu\delta_{ij}S_{kk}\right)\right)\right\} \tag{42}$$

Where the right hand side of (42) is from the Navier-Stoke equation (47).

Applying the time filtering operation $G(t-t')$ with a constant filter width on Equation (42) and using the sifting property of FG-PDF, we may obtain (noting that the differential commutation property of the time filtering operation is valid with a constant time filter width)

$$\frac{\partial F_U}{\partial t}+V_j\frac{\partial F_U}{\partial x_j}=-\frac{\partial}{\partial V_i}\left\{-\int_{-\infty}^{\infty}\rho f_U'\left(\frac{1}{\rho}\frac{\partial P}{\partial x_i}\right)G(t-t')\,dt'+\int_{-\infty}^{\infty}\rho f_U'\left(\frac{1}{\rho}\frac{\partial}{\partial x_j}\left(2\mu S_{ij}-\frac{2}{3}\mu\delta_{ij}S_{kk}\right)\right)G(t-t')\,dt'\right\}$$

According to Equation (41), the DW-FDF equation for the velocity can be written as

$$\frac{\partial F_U}{\partial t}+V_j\frac{\partial F_U}{\partial x_j}=-\frac{\partial}{\partial V_i}\left\{-F_U\cdot\left\langle\frac{1}{\rho}\frac{\partial P}{\partial x_i}\middle|\boldsymbol{V}\right\rangle_L+F_U\cdot\left\langle\frac{1}{\rho}\frac{\partial}{\partial x_j}\left(2\mu S_{ij}-\frac{2}{3}\mu\delta_{ij}S_{kk}\right)\middle|\boldsymbol{V}\right\rangle_L\right\} \tag{43}$$

At this point, the velocity DW-FDF equation is general but unclosed because of the unknown terms of the conditional DW-FDF means. The last term in Equation (43) is referred as the molecular mixing term and was modeled in various empirical ways by different researchers. Later, we will see that, when using a different way to derive the DW-FDF equation, the molecular mixing term is automatically closed with no need of modeling. The same happens to the pressure gradient term.

3.2 Traditional DW-FDF Equation for $F_\Phi(\boldsymbol{\psi}\,;\boldsymbol{x},t)$

Applying the time filtering $G(t-t')$ on the following FG-PDF equation for scalars,

$$\frac{\partial \rho f_\Phi'}{\partial t}+\frac{\partial \rho U_j f_\Phi'}{\partial x_j}=-\frac{\partial}{\partial \psi_i}\left\{f_\Phi'\left(\frac{\partial}{\partial x_j}\left(\rho\Gamma_{(i)}\frac{\partial \Phi_i}{\partial x_j}\right)+\rho S_i\left(\boldsymbol{\Phi}(\boldsymbol{x},t)\right)\right)\right\} \tag{44}$$

we obtain the DW-FDF equation for the turbulent species:

$$\frac{\partial F_\Phi}{\partial t}+\frac{\partial\left(F_\Phi\left\langle U_j\middle|\boldsymbol{\psi}\right\rangle_L\right)}{\partial x_j}=-\frac{\partial}{\partial \psi_i}\left\{F_\Phi\cdot\left\langle\frac{1}{\rho}\frac{\partial}{\partial x_j}\rho\Gamma_{(i)}\frac{\partial \Phi_i}{\partial x_j}\middle|\boldsymbol{\psi}\right\rangle_L+F_\Phi\cdot S_i\left(\boldsymbol{\psi}\right)\right\} \tag{45}$$

where $S_{N+1}(\boldsymbol{\psi}) = 0$. Equation (45) is also unclosed, because the conditional DW-FDF means need to be modeled. Later, we will also see that using a different derivation of DW-FDF equation, the molecular mixing term is closed.

4.0 DW-FDF Equations Derived From Filtered Navier-Stokes Equations

4.1 Filtered Compressible Navier-Stokes Equations

The Navier-Stokes equations for a compressible reacting flow can be written as

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho U_j}{\partial x_j} = 0 \tag{46}$$

$$\frac{\partial \rho U_i}{\partial t} + \frac{\partial \rho U_i U_j}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j}\left(2\rho\nu(S_{ij} - \frac{1}{3}\delta_{ij} S_{kk})\right) \tag{47}$$

$$\frac{\partial \rho e}{\partial t} + \frac{\partial \rho U_i e}{\partial x_i} = -\frac{\partial q_i}{\partial x_i} + P S_{kk} + 2\rho\nu\left(S_{ij} S_{ij} - \frac{1}{3} S_{ii} S_{kk}\right) + Q \tag{48}$$

$$\frac{\partial \rho \Phi_m}{\partial t} + \frac{\partial \rho U_i \Phi_m}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\rho \Gamma^{(m)} \frac{\partial \Phi_m}{\partial x_i}\right) + W_m \qquad m = 1, 2, \cdots, N \tag{49}$$

$$P = \rho R \sum_{n=1}^{N} \frac{\Phi_n T}{w_n} \tag{50}$$

$$q_i = -\rho \kappa c_\upsilon \frac{\partial T}{\partial x_i} - \sum_{m=1}^{N} \rho \Gamma^{(m)} h_m \frac{\partial \Phi_m}{\partial x_i} \tag{51}$$

Applying the time filtering operation with a constant filter width on the above equations, we obtain the following filtered Navier-Stokes equations:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \tilde{U}_j}{\partial x_j} = 0 \tag{52}$$

$$\frac{\partial \bar{\rho} \tilde{U}_i}{\partial t} + \frac{\partial \bar{\rho} \widetilde{U_i U_j}}{\partial x_j} = -\frac{\partial \bar{P}}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\overline{2\rho\nu(S_{ij} - \frac{1}{3}\delta_{ij} S_{kk})}\right) \tag{53}$$

$$\frac{\partial \bar{\rho} \tilde{e}}{\partial t} + \frac{\partial \bar{\rho} \widetilde{U_i e}}{\partial x_i} = -\frac{\partial \bar{q}_i}{\partial x_i} + \overline{P S_{kk}} + \overline{2\rho\nu\left(S_{ij} S_{ij} - \frac{1}{3} S_{ii} S_{kk}\right)} + \bar{Q} \tag{54}$$

$$\frac{\partial \bar{\rho} \tilde{\Phi}_m}{\partial t} + \frac{\partial \bar{\rho} \widetilde{U_i \Phi_m}}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\overline{\rho \Gamma^{(m)} \frac{\partial \Phi_m}{\partial x_i}}\right) + \bar{W}_m \qquad m = 1, 2, \cdots, N \tag{55}$$

where

$$\overline{P} = \overline{\rho} R \sum_{n=1}^{N} \frac{\widetilde{\Phi_n T}}{w_n} = \frac{\overline{\rho} R}{c_v} \sum_{n=1}^{N} \frac{\widetilde{\Phi_n e}}{w_n}$$

or (56)

$$\overline{P} = \frac{\overline{\rho} R}{c_v} \sum_{n=1}^{N} \frac{\widetilde{\Phi_n \Phi_{N+1}}}{w_n}$$

$$\overline{q}_i = -\overline{\rho \kappa c_\upsilon \frac{\partial T}{\partial x_i}} - \sum_{m=1}^{N} \overline{\rho \Gamma^{(m)} h_m \frac{\partial \Phi_m}{\partial x_i}} \tag{57}$$

In the above equations, κ, ν and $\Gamma^{(m)}$ are the molecular heat conductivity, kinematic viscosity and the *m*-th species diffusivity, they have the same dimension (i.e., velocity · length). The h_m, T are the enthalpy of species and temperature, Q is the radiation rate, $W_m = \rho S_m$ is the chemical generation rate of the *m*-th species, Φ_{N+1} represents the internal energy e, R is the universal gas constant. These equations are general; however, unlike the constant density flows, further approximations for the terms on their right hand side are required in order to complete the filtering process. One of such approximations leads to

$$\overline{2\rho\nu\left(S_{ij} - \frac{1}{3}\delta_{ij} S_{kk}\right)} \approx \mu\left(\frac{\partial \tilde{U}_i}{\partial x_j} + \frac{\partial \tilde{U}_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial \tilde{U}_k}{\partial x_k}\right) \tag{58}$$

In which, we have basically neglected the variations of μ and ρduring the filtering process, the value of μ will be considered as the function of $\overline{P}, \tilde{T}, \cdots$. Another type of approximation writes

$$\overline{2\rho\nu\left(S_{ij} - \frac{1}{3}\delta_{ij} S_{kk}\right)} \approx \nu\left(\frac{\partial \overline{\rho} \tilde{U}_i}{\partial x_j} + \frac{\partial \overline{\rho} \tilde{U}_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial \overline{\rho} \tilde{U}_k}{\partial x_k}\right) \tag{59}$$

Similarly,

$$\overline{q}_i = -\overline{\rho \kappa c_\upsilon \frac{\partial T}{\partial x_i}} - \sum_{m=1}^{N} \overline{\rho \Gamma^{(m)} h_m \frac{\partial \Phi_m}{\partial x_i}} \approx -\kappa c_\upsilon \frac{\partial \overline{\rho} \tilde{T}}{\partial x_i} - \sum_{m=1}^{N} \Gamma^{(m)} \frac{\partial \overline{\rho} \widetilde{h_m \Phi_m}}{\partial x_i} \tag{60}$$

$$\overline{\rho \Gamma^{(m)} \frac{\partial \Phi_m}{\partial x_i}} \approx \Gamma^{(m)} \frac{\partial \overline{\rho} \tilde{\Phi}_m}{\partial x_i} \tag{61}$$

Furthermore, invoking the turbulent kinetic energy dissipation rate:

$$\overline{2\rho\nu\left(S_{ij} S_{ij} - \frac{1}{3} S_{ii} S_{kk}\right)} \equiv \overline{\rho}\,\tilde{\varepsilon} \tag{62}$$

Where ν, κ, c_υ and $\Gamma^{(m)}$ are considered as the function of $\overline{P}, \tilde{T}, \cdots$.

Therefore, the filtered Navier-Stokes equations can approximately be written as

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \overline{\rho} \tilde{U}_j}{\partial x_j} = 0 \tag{63}$$

$$\frac{\partial \bar{\rho}\tilde{U}_i}{\partial t}+\frac{\partial \bar{\rho}\widetilde{U_i U_j}}{\partial x_j}=-\frac{\partial \bar{P}}{\partial x_i}+\frac{\partial}{\partial x_j}\left[\nu\left(\frac{\partial \bar{\rho}\tilde{U}_i}{\partial x_j}+\frac{\partial \bar{\rho}\tilde{U}_j}{\partial x_i}-\frac{2}{3}\delta_{ij}\frac{\partial \bar{\rho}\tilde{U}_k}{\partial x_k}\right)\right] \tag{64}$$

$$\frac{\partial \bar{\rho}\tilde{e}}{\partial t}+\frac{\partial \bar{\rho}\widetilde{U_i e}}{\partial x_i}=-\frac{\partial \bar{q}_i}{\partial x_i}+\overline{PS_{kk}}+\bar{\rho}\tilde{\varepsilon}+\bar{Q} \tag{65}$$

$$\frac{\partial \bar{\rho}\tilde{\Phi}_m}{\partial t}+\frac{\partial \bar{\rho}\widetilde{U_i\Phi_m}}{\partial x_i}=\frac{\partial}{\partial x_i}\left(\Gamma^{(m)}\frac{\partial \bar{\rho}\tilde{\Phi}_m}{\partial x_i}\right)+\bar{\rho}\tilde{S}_m \qquad m=1,2,\cdots,N \tag{66}$$

$$\bar{P}=\bar{\rho}R\sum_{n=1}^{N}\frac{\widetilde{\Phi_n T}}{w_n}=\frac{\bar{\rho}R}{c_v}\sum_{n=1}^{N}\frac{\widetilde{\Phi_n e}}{w_n}$$

or (67)

$$\bar{P}=\frac{\bar{\rho}R}{c_v}\sum_{n=1}^{N}\frac{\widetilde{\Phi_n\Phi_{N+1}}}{w_n}$$

$$\bar{q}_i=-\kappa c_\upsilon\frac{\partial \bar{\rho}\tilde{T}}{\partial x_i}-\sum_{m=1}^{N}\Gamma^{(m)}\frac{\partial \bar{\rho}\widetilde{h_m\Phi_m}}{\partial x_i} \tag{68}$$

These equations are still considered as quite general, because i) they are exact if the flow becomes incompressible, ii) all the approximations made in Equations (64), (65) and (66) are related only to the molecular diffusion terms that are less important and even negligible comparing with the convection terms on the left hand side for turbulent flows at high Reynolds number (see Tennekes and Lumley (Ref. 7) and Pope (Ref. 3)). For the LES simulation, Equation (63) to (66) are often used together with the further approximations for (67) and (68):

$$\bar{P}=\overline{\rho R\sum_{n=1}^{N}\frac{\Phi_n T}{w_n}}=\overline{\left(\frac{\rho RT}{M}\right)}\approx\frac{\bar{\rho}R\tilde{T}}{\bar{M}},\quad \bar{M}=\sum_{n=1}^{N}\frac{\tilde{\Phi}_n}{w_n} \tag{69}$$

$$\bar{q}_i=-\kappa c_\upsilon\frac{\partial \bar{\rho}\tilde{T}}{\partial x_i} \tag{70}$$

The momentum flux $\bar{\rho}\widetilde{U_iU_j}$, the energy flux $\bar{\rho}\widetilde{U_ie}$ and the species flux $\bar{\rho}\widetilde{U_i\Phi_m}$ are considered to be critically important in LES simulations and should be carefully modeled. Many models in the literature, from the simplest Smagorinsky (Ref. 8) model to the complex two-equation models (Refs. 9 and 6) including the dynamic procedure (Ref. 10) have been suggested. In the next Section 4.2 and 4.3, we will derive the DW-FDF equations directly from Equations (63) to (68).

4.2 DW-FDF Equation for $F_U(\boldsymbol{V};x,t)$

Using Equations (28) and (33), the left hand side of Equation (64) can be written as

$$\frac{\partial \bar{\rho}\tilde{U}_i}{\partial t}+\frac{\partial \bar{\rho}\widetilde{U_iU_j}}{\partial x_j}=\frac{\partial}{\partial t}\int_{-\infty}^{\infty}V_i F_U\,d\boldsymbol{V}+\frac{\partial}{\partial x_j}\int_{-\infty}^{\infty}V_iV_j F_U\,d\boldsymbol{V}=\int_{-\infty}^{\infty}V_i\left(\frac{\partial F_U}{\partial t}+V_j\frac{\partial F_U}{\partial x_j}\right)d\boldsymbol{V} \tag{71}$$

The pressure gradient term can be written as using (67)

$$-\frac{\partial \overline{P}}{\partial x_i} = -\frac{\partial}{\partial x_i}\left(\frac{\overline{\rho} R}{c_v}\sum_{n=1}^{N}\widetilde{\frac{\Phi_n \Phi_{N+1}}{w_n}}\right) = \begin{cases} \int_{-\infty}^{\infty} V_i \frac{\partial^2}{\partial V_k \partial x_k}\left[\sum_{n=1}^{N}\frac{R}{c_v w_n}\left(\int_{-\infty}^{\infty}\psi_n \psi_{N+1} F_{U,\Phi}(\boldsymbol{\psi},\boldsymbol{V};x,t)d\boldsymbol{\psi}\right)\right] d\boldsymbol{V} \\ \text{or} \\ \int_{-\infty}^{\infty} V_i \frac{\partial^2}{\partial V_k \partial x_k}\left[\sum_{n=1}^{N}\frac{R}{c_v w_n}\left\langle \Phi_n \Phi_{N+1} \middle| \boldsymbol{V}\right\rangle_L F_U\right] d\boldsymbol{V} \end{cases} \tag{72}$$

During the above arrangement, no approximations have been made other than the integration by parts and a zero integration property like Eq.(74).

Note that the pressure gradient term can be closed only when the joint DW-FDF, $F_{U,\Phi}$, is considered, otherwise, the "conditional DW-FDF mean" will be unavoidable. Now the molecular mixing term in Equation (64) can be written as

$$\begin{aligned} &\frac{\partial}{\partial x_j}\nu\left(\frac{\partial \overline{\rho}\tilde{U}_i}{\partial x_j} + \frac{\partial \overline{\rho}\tilde{U}_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial \overline{\rho}\tilde{U}_m}{\partial x_m}\right) \\ &= \frac{\partial}{\partial x_j}\nu\left(\frac{\partial}{\partial x_j}\int_{-\infty}^{\infty} V_i F_U\, d\boldsymbol{V} + \frac{\partial}{\partial x_i}\int_{-\infty}^{\infty} V_j F_U\, d\boldsymbol{V} - \frac{2}{3}\delta_{ij}\frac{\partial}{\partial x_m}\int_{-\infty}^{\infty} V_m F_U\, d\boldsymbol{V}\right) \\ &= \begin{cases} \int_{-\infty}^{\infty} V_i\left(\frac{\partial}{\partial x_j}\nu\frac{\partial F_U}{\partial x_j}\right) d\boldsymbol{V} - \frac{\partial}{\partial x_j}\nu\left(\frac{\partial}{\partial x_k}\int_{-\infty}^{\infty} V_i \frac{\partial}{\partial V_k}\left(V_j F_U\right) d\boldsymbol{V} - \frac{2}{3}\delta_{kj}\frac{\partial}{\partial x_m}\int_{-\infty}^{\infty} V_i \frac{\partial}{\partial V_k}\left(V_m F_U\right) d\boldsymbol{V}\right) \\ \text{or} \\ -\frac{\partial}{\partial x_j}\nu\left(\frac{\partial}{\partial x_j}\int_{-\infty}^{\infty} V_i \frac{\partial}{\partial V_k}\left(V_k F_U\right) d\boldsymbol{V} + \frac{\partial}{\partial x_k}\int_{-\infty}^{\infty} V_i \frac{\partial}{\partial V_k}\left(V_j F_U\right) d\boldsymbol{V} - \frac{2}{3}\delta_{kj}\frac{\partial}{\partial x_m}\int_{-\infty}^{\infty} V_i \frac{\partial}{\partial V_k}\left(V_m F_U\right) d\boldsymbol{V}\right) \end{cases} \\ &= \begin{cases} \int_{-\infty}^{\infty} V_i\left(\frac{\partial}{\partial x_j}\nu\frac{\partial F_U}{\partial x_j}\right) d\boldsymbol{V} - \int_{-\infty}^{\infty} V_i \frac{\partial}{\partial x_j}\left(\nu\frac{\partial^2 V_j F_U}{\partial V_k \partial x_k}\right) d\boldsymbol{V} + \int_{-\infty}^{\infty} V_i \frac{2}{3}\delta_{kj}\frac{\partial}{\partial x_j}\left(\nu\frac{\partial^2 V_m F_U}{\partial V_k \partial x_m}\right) d\boldsymbol{V} \\ \text{or} \\ -\int_{-\infty}^{\infty} V_i \frac{\partial}{\partial x_j}\left(\nu\frac{\partial^2 V_k F_U}{\partial V_k \partial x_j}\right) d\boldsymbol{V} - \int_{-\infty}^{\infty} V_i \frac{\partial}{\partial x_j}\left(\nu\frac{\partial^2 V_j F_U}{\partial V_k \partial x_k}\right) d\boldsymbol{V} + \int_{-\infty}^{\infty} V_i \frac{2}{3}\delta_{kj}\frac{\partial}{\partial x_j}\left(\nu\frac{\partial^2 V_m F_U}{\partial V_k \partial x_m}\right) d\boldsymbol{V} \end{cases} \end{aligned} \tag{73}$$

Note, on the third line of (73), we have applied the integration by parts and the following type of zero integration similar to the one used in PDF formulations (Ref. 3):

$$\int_{-\infty}^{\infty} \frac{\partial}{\partial V_k}\left(V_i V_k F_U\right) d\boldsymbol{V} = 0 \tag{74}$$

Finally, collecting the terms that are in the integrands and factored by V_i, we obtain the transport equation for $F_U(\boldsymbol{V}; \boldsymbol{x},t)$ as

$$\frac{\partial F_U}{\partial t}+V_j\frac{\partial F_U}{\partial x_j}=\frac{\partial^2}{\partial V_k\partial x_k}\left[\sum_{n=1}^{N}\frac{R}{c_v w_n}\left\langle \Phi_n\Phi_{N+1}\middle|\boldsymbol{V}\right\rangle_L F_U\right]+\frac{\partial}{\partial x_j}\left(\nu\frac{\partial F_U}{\partial x_j}\right)$$
$$-\frac{\partial}{\partial V_k}\left(V_j\frac{\partial}{\partial x_j}\nu\frac{\partial F_U}{\partial x_k}\right)+\frac{\partial}{\partial V_k}\left(\frac{2}{3}\delta_{kj}V_m\frac{\partial}{\partial x_j}\nu\frac{\partial F_U}{\partial x_m}\right)$$

or (75)

$$\frac{\partial F_U}{\partial t}+V_j\frac{\partial F_U}{\partial x_j}=\frac{\partial^2}{\partial V_k\partial x_k}\left[\sum_{n=1}^{N}\frac{R}{c_v w_n}\left\langle \Phi_n\Phi_{N+1}\middle|\boldsymbol{V}\right\rangle_L F_U\right]-\frac{\partial}{\partial V_k}\left(V_k\frac{\partial}{\partial x_j}\nu\frac{\partial F_U}{\partial x_j}\right)$$
$$-\frac{\partial}{\partial V_k}\left(V_j\frac{\partial}{\partial x_j}\nu\frac{\partial F_U}{\partial x_k}\right)+\frac{\partial}{\partial V_k}\left(\frac{2}{3}\delta_{kj}V_m\frac{\partial}{\partial x_j}\nu\frac{\partial F_U}{\partial x_m}\right)$$

In Equation (75), all the terms are closed, except for the one involving the conditional DW-FDF mean originating from the pressure gradient. It should be noticed that one of the most important terms in the momentum equation, i.e., $\overline{\rho}\widetilde{U_iU_j}$, now is closed in the corresponding DW-FDF equation. And the less important molecular diffusion terms remain in the closed form.

4.3 DW-FDF Equation for $F_\Phi(\boldsymbol{\psi};\boldsymbol{x},t)$

Similarly, we may obtain the DW-FDF equations for the scalars (i.e. species and internal energy) from Equations (65), (66) as follows: first, we write the terms on the left hand side of Equation (66) as

$$\frac{\partial\overline{\rho}\,\widetilde{\Phi}_m}{\partial t}=\frac{\partial}{\partial t}\int_{-\infty}^{\infty}\psi_m F_\Phi\,d\boldsymbol{\psi}=\int_{-\infty}^{\infty}\psi_m\frac{\partial F_\Phi}{\partial t}d\boldsymbol{\psi} \tag{76}$$

$$\frac{\partial\overline{\rho}\,\widetilde{U_i\Phi_m}}{\partial x_i}=\frac{\partial}{\partial x_i}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}V_i\,\psi_m F_{U,\Phi}\,d\boldsymbol{V}d\boldsymbol{\psi}=\begin{cases}\displaystyle\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\psi_m\left(V_i\frac{\partial}{\partial x_i}F_{U,\Phi}\right)d\boldsymbol{V}\,d\boldsymbol{\psi}\\ \text{or}\\ \displaystyle\int_{-\infty}^{\infty}\psi_m\left(\frac{\partial}{\partial x_i}\left(F_\Phi\left\langle U_i\middle|\boldsymbol{\psi}\right\rangle_L\right)\right)d\boldsymbol{\psi}\end{cases} \tag{77}$$

Then, the terms on the right hand side of (66) can be written as

$$\frac{\partial}{\partial x_i}\left(\Gamma^{(m)}\frac{\partial\overline{\rho}\,\widetilde{\Phi}_m}{\partial x_i}\right)=\frac{\partial}{\partial x_i}\left(\Gamma^{(m)}\frac{\partial}{\partial x_i}\int_{-\infty}^{\infty}\psi_m F_\Phi\,d\boldsymbol{\psi}\right)=\begin{cases}\displaystyle\int_{-\infty}^{\infty}\psi_m\frac{\partial}{\partial x_i}\left(\Gamma^{(m)}\frac{\partial F_\Phi}{\partial x_i}\right)d\boldsymbol{\psi}\\ \text{or}\\ \displaystyle-\int_{-\infty}^{\infty}\psi_m\frac{\partial}{\partial x_i}\left(\Gamma^{(m)}\frac{\partial^2\psi_k F_\Phi}{\partial\psi_k\partial x_i}\right)d\boldsymbol{\psi}\end{cases} \tag{78}$$

$$\bar{\rho}\tilde{S}_m = \int_{-\infty}^{\infty} S_m(\boldsymbol{\psi}) F_\Phi d\boldsymbol{\psi} = -\int_{-\infty}^{\infty} \psi_m \frac{\partial\left(S_k F_\Phi\right)}{\partial\psi_k} d\boldsymbol{\psi} \tag{79}$$

Where in Equations (78) and (79), we have applied the integration by parts and zero integrations similar to (74). Collecting all the integrand terms that factored by ψ_m, we obtain

$$\frac{\partial F_\Phi}{\partial t} + \frac{\partial\left(F_\Phi \left\langle U_i \middle| \boldsymbol{\psi}\right\rangle_L\right)}{\partial x_i} = \left\{\frac{\partial}{\partial x_i}\left(\Gamma^{(m)} \frac{\partial F_\Phi}{\partial x_i}\right) - \frac{\partial}{\partial\psi_k}\left[F_\Phi \cdot S_k\left(\boldsymbol{\psi}\right)\right]\right\}, \quad m = 1, 2, \cdots, N+1$$

or (80)

$$\frac{\partial F_\Phi}{\partial t} + \frac{\partial\left(F_\Phi \left\langle U_i \middle| \boldsymbol{\psi}\right\rangle_L\right)}{\partial x_i} = -\frac{\partial}{\partial\psi_k}\left\{\frac{\partial}{\partial x_i}\left(\Gamma^{(m)} \psi_k \frac{\partial F_\Phi}{\partial x_i}\right) + F_\Phi \cdot S_k\left(\boldsymbol{\psi}\right)\right\}, \quad m = 1, 2, \cdots, N+1$$

This equation also represents the equation of internal energy $m = N + 1$, where $S_{N+1}(\boldsymbol{\psi}) = 0$ and other source terms in Equation (65) are neglected as suggested by Jaberi et al. (Ref. 1). Equation (80) is essentially closed if we consider the joint DW-FDF $F_{U,\Phi}$. For the marginal F_Φ, the convection term is not closed because of the conditional DW-FDF mean $\left\langle U_i \middle| \boldsymbol{\psi}\right\rangle_L$. Then, this critically important term, corresponding to $\bar{\rho}\widetilde{U_i\Phi_m}$ in Equation (66), must be carefully modeled while the less important molecular diffusion term remains in the closed form. In addition, we noticed that the equally important chemistry source term $\bar{\rho}\widetilde{S_m(\boldsymbol{\Phi})}$ in Equation (66) contains complex processes of turbulence-chemistry interaction, which is considered as very hard to be modeled. However, it is closed in the DW-FDF equation with no need of modeling. This direct calculation of turbulence-chemistry interaction represents one of the unique features of DW-FDF methodology.

4.4 Modeling of Unclosed Terms

Consider the approximation described by Equation (69), i.e. $\bar{P} \approx \bar{\rho}R\tilde{T}/\bar{M}$, we may write from Equation (72)

$$\begin{aligned}
-\frac{\partial\bar{P}}{\partial x_i} &= -\frac{\partial}{\partial x_i}\left(\frac{\bar{\rho}R}{c_v}\sum_{n=1}^{N}\frac{\widetilde{\Phi_n\Phi_{N+1}}}{w_n}\right) \approx -\frac{\partial}{\partial x_i}\left(\frac{\bar{\rho}R\,\tilde{\Phi}_{N+1}}{c_v\bar{M}}\right) \\
&= -\frac{\partial}{\partial x_i}\frac{R}{c_v\bar{M}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\psi_{N+1}F_{U,\Phi}\,d\boldsymbol{\psi}\,d\boldsymbol{V} \\
&= -\frac{\partial}{\partial x_i}\frac{R}{c_v\bar{M}}\int_{-\infty}^{\infty}\left\langle \Phi_{N+1} \middle| \boldsymbol{V}\right\rangle_L F_U\,d\boldsymbol{V} \\
&= \int_{-\infty}^{\infty} V_i \frac{\partial^2}{\partial V_k \partial x_k}\left[\frac{R}{c_v\bar{M}}\left\langle \Phi_{N+1} \middle| \boldsymbol{V}\right\rangle_L F_U\right] d\boldsymbol{V} \\
&\approx \int_{-\infty}^{\infty} V_i \frac{\partial^2}{\partial V_k \partial x_k}\left[\frac{R\,\tilde{e}}{c_v\bar{M}} F_U\right] d\boldsymbol{V}
\end{aligned} \tag{81}$$

The last step in Equation (81) employs a rough approximation:

$$\left\langle \Phi_{N+1} \middle| \boldsymbol{V} \right\rangle_L \approx \tilde{\Phi}_{N+1} = \tilde{e} \tag{82}$$

As for the convection term in the species Equation (80), $F_\Phi \left\langle U_i \middle| \boldsymbol{\psi} \right\rangle_L$, we may start from a more general model for the term $\overline{\rho}\widetilde{U_i \Phi_m}$ (see Ref. 6):

$$\overline{\rho}\widetilde{U_i \Phi_m} = \overline{\rho}\tilde{U}_i \tilde{\Phi}_m - \Gamma_T^{(m)} \frac{\partial \overline{\rho}\tilde{\Phi}_m}{\partial x_i} - \Gamma_T^{(m)} \frac{k}{\varepsilon}\left(c_1 \widetilde{S}_{ij} + c_2 \widetilde{\Omega}_{ij}\right)\frac{\partial \overline{\rho}\tilde{\Phi}_m}{\partial x_j} \tag{83}$$

Where $c_1 = c_2 = -0.24$. This will lead to the following model by directly applying the Equations (27) and (39) described in Sections 2.2.2 and 2.2.3:

$$F_\Phi \left\langle U_i \middle| \boldsymbol{\psi} \right\rangle_L = \widetilde{U}_i F_\Phi - \left[\Gamma_T^{(m)} \frac{\partial F_\Phi}{\partial x_i}\right] + \frac{\partial}{\partial \psi_k}\left[\Gamma_T^{(m)} \frac{k}{\varepsilon}\left(c_1 \widetilde{S}_{ij} + c_2 \widetilde{\Omega}_{ij}\right)\psi_k \frac{\partial F_\Phi}{\partial x_j}\right]$$

or (84)

$$F_\Phi \left\langle U_i \middle| \boldsymbol{\psi} \right\rangle_L = \widetilde{U}_i F_\Phi + \frac{\partial}{\partial \psi_k}\left[\Gamma_T^{(m)} \psi_k \frac{\partial F_\Phi}{\partial x_i}\right] + \frac{\partial}{\partial \psi_k}\left[\Gamma_T^{(m)} \frac{k}{\varepsilon}\left(c_1 \widetilde{S}_{ij} + c_2 \widetilde{\Omega}_{ij}\right)\psi_k \frac{\partial F_\Phi}{\partial x_j}\right]$$

4.5 Summary

With the models given by Equations (81) and (84), the marginal DW-FDF equations for $F_U(\boldsymbol{V}; \boldsymbol{x},\boldsymbol{t})$ and $F_\Phi(\boldsymbol{\psi}; \boldsymbol{x},\boldsymbol{t})$ can be written as

$$\frac{\partial F_U}{\partial t} + V_j \frac{\partial F_U}{\partial x_j} = \frac{\partial^2}{\partial V_k \partial x_k}\left[\frac{R\tilde{\Phi}_{N+1}}{c_v \bar{M}} F_U\right] + \frac{\partial}{\partial x_j}\left(\nu \frac{\partial F_U}{\partial x_j}\right) - \frac{\partial}{\partial V_k}\left(V_j \frac{\partial}{\partial x_j}\nu \frac{\partial F_U}{\partial x_k}\right) + \frac{\partial}{\partial V_k}\left(\frac{2}{3}\delta_{kj} V_m \frac{\partial}{\partial x_j}\nu \frac{\partial F_U}{\partial x_m}\right)$$

or (85)

$$\frac{\partial F_U}{\partial t} + V_j \frac{\partial F_U}{\partial x_j} = \frac{\partial^2}{\partial V_k \partial x_k}\left[\frac{R\tilde{\Phi}_{N+1}}{c_v \bar{M}} F_U\right] - \frac{\partial}{\partial V_k}\left(V_k \frac{\partial}{\partial x_j}\nu \frac{\partial F_U}{\partial x_j}\right) - \frac{\partial}{\partial V_k}\left(V_j \frac{\partial}{\partial x_j}\nu \frac{\partial F_U}{\partial x_k}\right) + \frac{\partial}{\partial V_k}\left(\frac{2}{3}\delta_{kj} V_m \frac{\partial}{\partial x_j}\nu \frac{\partial F_U}{\partial x_m}\right)$$

$$
\frac{\partial F_{\Phi}}{\partial t}+\frac{\partial\left(\widetilde{U}_i F_{\Phi}\right)}{\partial x_i}=\left\{\frac{\partial}{\partial x_i}\left(\left(\Gamma^{(m)}+\Gamma_T^{(m)}\right)\frac{\partial F_{\Phi}}{\partial x_i}\right)\right\}-\frac{\partial}{\partial \psi_k}\left(F_{\Phi}\cdot S_k\left(\boldsymbol{\psi}\right)\right)
$$

$$
-\frac{\partial}{\partial \psi_k}\left\{\psi_k\frac{\partial}{\partial x_i}\left(\Gamma_T^{(m)}\frac{k}{\varepsilon}\left(c_1\widetilde{S}_{ij}+c_2\widetilde{\Omega}_{ij}\right)\frac{\partial F_{\Phi}}{\partial x_j}\right)\right\}, \qquad m=1,2,\cdots,N+1
$$

or (86)

$$
\frac{\partial F_{\Phi}}{\partial t}+\frac{\partial\left(\widetilde{U}_i F_{\Phi}\right)}{\partial x_i}=-\frac{\partial}{\partial \psi_k}\left\{\psi_k\frac{\partial}{\partial x_i}\left(\left(\Gamma^{(m)}+\Gamma_T^{(m)}\right)\frac{\partial F_{\Phi}}{\partial x_i}\right)+F_{\Phi}\cdot S_k\left(\boldsymbol{\psi}\right)\right\}
$$

$$
-\frac{\partial}{\partial \psi_k}\left\{\psi_k\frac{\partial}{\partial x_i}\left(\Gamma_T^{(m)}\frac{k}{\varepsilon}\left(c_1\widetilde{S}_{ij}+c_2\widetilde{\Omega}_{ij}\right)\frac{\partial F_{\Phi}}{\partial x_j}\right)\right\}, \qquad m=1,2,\cdots,N+1
$$

It can be verified that the DW-FDF Equations (85) and (86) can exactly deduce the filtered compressible Navier-Stoke equations (64) to (66) with the assumed approximations of (81) and (83). However, by no means, the models described by Equations (81) and (84) are unique. Furthermore, the variables ($\tilde{\Phi}_{N+1}$, $\tilde{U}_i$, $\tilde{S}_{ij}$ and $\tilde{\Omega}_{ij}$) are considered as available during the solution procedure of the DW-FDF equations.

5.0 Concluding Remarks

We have revisited the derivations of the traditional DW-FDF or FMDF equations by starting from the equation of FG-PDF that contains all the terms on the right hand side of the Navier-Stokes equations, see Equations (42) and (44). The resulting FMDF equations contain the "conditional DW-FDF mean" quantities for all the terms on the right hand side (except for the reaction term), see Equations (43), (45), which need empirical models to make the equations closed.

From the relationship between the DW-FDF and the filtered turbulent variables, it is possible to construct the DW-FDF equations directly from the filtered compressible Navier-Stokes equations. Such DW-FDF equations have an outstanding feature that all the terms that were not closed on the right hand side of traditional FMDF equations are now in the closed form, see Equations (75) and (80), except for the pressure gradient term that involves joint DW-FDF.

In the marginal DW-FDF equations, the two unclosed terms, one related to the pressure gradient and the other related to the species convection, are expected to be more important than the molecular "mixing" or "diffusion" terms, especially in the case of high Reynolds number. Their physics-based models, such as Equations (81) and (84), should be further developed and evaluated.

The fundamental differences between the DW-FDF (a random quantity) and the PDF (a deterministic quantity) warrant further investigation on their respective solution procedure using the stochastic differential equation methods.

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14. ABSTRACT In this report, we briefly revisit the formulation of density weighted filtered density function (DW-FDF) for large eddy simulation (LES) of turbulent reacting flows, which was proposed by Jaberi et al. (Jaberi, F.A., Colucci, P.J., James, S., Givi, P. and Pope, S.B., “Filtered mass density function for Large-eddy simulation of turbulent reacting flows,” J. Fluid Mech., vol. 401, pp. 85-121, 1999). At first, we proceed the traditional derivation of the DW-FDF equations by using the fine grained probability density function (FG-PDF), then we explore another way of constructing the DW-FDF equations by starting directly from the compressible Navier-Stokes equations. We observe that the terms which are unclosed in the traditional DW-FDF equations are now closed in the newly constructed DW-FDF equations. This significant difference and its practical impact on the computational simulations may deserve further studies.						
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