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Conservational PDF Equations of Turbulence

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Abstract

Recently we have revisited the traditional probability density function (PDF) equations for the velocity and species in turbulent incompressible flows. They are all unclosed due to the appearance of various conditional means which are modeled empirically. However, we have observed that it is possible to establish a closed velocity PDF equation and a closed joint velocity and species PDF equation through conditions derived from the integral form of the Navier-Stokes equations. Although, in theory, the resulted PDF equations are neither general nor unique, they nevertheless lead to the exact transport equations for the first moment as well as all higher order moments. We refer these PDF equations as the conservational PDF equations. This observation is worth further exploration for its validity and CFD application.

1.0 Introduction

To explore the turbulence modeling employed in the PDF method, we revisited the constructions of the traditional PDF equations for turbulent velocity and species, which were described by several researchers in great details, for example, by Pope (Ref. 1). In those constructions, a Delta function (which is referred as the fine grained PDF) was extensively used, together with a few impressive mathematical techniques to invoke the Navier-Stoke equations into the identity relationship developed from the Delta function. Since the entry point for the Navier-Stokes equations was through the "conditional mean", two or three conditional means appeared in the velocity PDF equation and additional two conditional means appeared in the species PDF equation. In these traditional PDF equations, all the conditional means were considered as unknowns and modeled empirically.

In the present study, we started out by taking the statistical mean directly on the Navier-Stokes equations to form an integral equation, from which a PDF equation is then constructed. Depending on the way of taking mean on some particular terms, especially the pressure gradient ∇P and the molecular diffusions $\nu\nabla^2 U_i$, $\Gamma\nabla^2\Phi_i$, the resulted PDF equation can end up with different forms. Briefly speaking, if we treat, for example, the molecular diffusion term $\nu\nabla^2 U_i$ as a separate random variable from U_i, then its mean $\left\langle \nu\nabla^2 U_i \right\rangle$ will be expressed as an integration of the product of the velocity PDF and the conditional mean, i.e.,

$$\left\langle \nu\nabla^2 U_i \right\rangle = \int \nu \left\langle \nabla^2 U_i \middle| \boldsymbol{V} \right\rangle f\left(\boldsymbol{V}\,;\,\boldsymbol{x},t\right) d\boldsymbol{V} \,,$$

where the conditional mean $\left\langle \nu\nabla^2 U_i \middle| V \right\rangle$ is a new unknown. However, if we take the mean based on the definition and the commutation rule between mean and differentiation, then we have

$$\left\langle \nu\nabla^2 U_i \right\rangle = \nu\nabla^2 \left\langle U_i \right\rangle = \nu\nabla^2 \int V_i\, f\left(\boldsymbol{V}\,;\,\boldsymbol{x},t\right) d\boldsymbol{V} = \int \nu \left(V_i \frac{\nabla^2 f}{f} \right) f\left(\boldsymbol{V}\,;\,\boldsymbol{x},t\right) d\boldsymbol{V} \,,$$

which is in closed form. The former way will lead to the traditional PDF equations (see Sections 3.3 and 4.2). The latter way will lead to the closed equations for the velocity PDF (see Section 3.4) and the joint species-velocity PDF (see Section 4.3). Since a sufficient but not necessary condition was involved in their construction, the resulted PDF equations are neither general nor unique. Nevertheless, we observed that they can lead to the exact transport equations for not only the first moments (i.e. mean velocity and species, etc.) but also all higher order moments deduced from the Navier-Stokes equations. This feature is referred as the conservation of the PDF equations.

Later, we also found that, for the traditional way of utilizing the “fine grained PDF”, all the conditional means (e.g., $\left\langle \nu \nabla^2 U_i \middle| \mathbf{V} \right\rangle, \left\langle \nu \nabla^2 \Phi_i \middle| \boldsymbol{\psi} \right\rangle$, etc.) can also be systematically modeled through similar sufficient condition, hence the traditional PDF equations can be closed exactly as the PDF equations proposed in the present study. The details are described in the Appendix A.

Section 2.0 introduces the basic definition of probability density function of turbulent velocity, species, other turbulent quantities and their joint PDF; the relationships between the marginal PDF, the joint PDF and the conditional PDF; and the relationship between the mean and the conditional mean. Section 3.0 demonstrates how to construct the velocity PDF equation starting directly from the Navier-Stokes equations. Section 4.0 demonstrates the construction of the transport equations for the species PDF and the joint species-velocity PDF.

2.0 PDF of Turbulent Variables

2.1 PDF of Turbulent Velocity $f_U(\boldsymbol{V}; \boldsymbol{x},t)$

Turbulent velocity $U_i(x_i,t)$ is a random vector variable, its probability density function PDF at a single point (in space and time) is denoted as $f_U(\boldsymbol{V}; \boldsymbol{x},t) \equiv f_U(V_1,V_2,V_3\,; x_1,x_2,x_3,t)$, where $\boldsymbol{V} \equiv (V_1,V_2,V_3)$ is the sample space coordinates of U_i, and $\boldsymbol{x} \equiv (x_1,x_2,x_3), t$ are the location coordinates and the time. Formally, $f_U(\boldsymbol{V}; \boldsymbol{x},t)$ is a scalar function of $\boldsymbol{V}$ and $\boldsymbol{x},t$, but its arguments have different physical meaning and mathematical transformation. The $\boldsymbol{V}$ represents a point in the velocity sample space ($-\infty < V_i < \infty, \quad i = 1, 2, 3$) at which the probability density f_U of U_i is defined. The $\boldsymbol{x},t$ indicate that f_U is a field and a process. It is important to note that $\boldsymbol{V}$ is independent of $\boldsymbol{x}$ and t. The probability density function $f_U(\boldsymbol{V}\,; \boldsymbol{x},t)$ itself is not random and is fully defined at each $\boldsymbol{V}$ for every single point $\boldsymbol{x},t$, it is a differentiable (hence continuous) function of $\boldsymbol{V}$, $\boldsymbol{x}$, t. Furthermore, its integration over the whole sample space $\boldsymbol{V}$ at every single point $\boldsymbol{x},t$ must be equal to one, because the total probability for all events must be 100 percent, i.e.,

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f_U(V_1,V_2,V_3\,; x_1,x_2,x_3,t)\, dV_1 dV_2 dV_3 = 1 . \tag{1}$$

Or written as

$$\int f_U(\boldsymbol{V}; \boldsymbol{x},t)\, d\boldsymbol{V} = 1 . \tag{2}$$

Where $\int (\quad) d\boldsymbol{V}$ is an abbreviation of $\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} (\quad)\, dV_1 dV_2 dV_3$. It is also important to note that the argument $\boldsymbol{V}$ in f_U represents ‘V_1,V_2,V_3’ so that $f_U(\boldsymbol{V}; \boldsymbol{x},t)$ is a joint probability density function $f_U(V_1,V_2,V_3\,; \boldsymbol{x},t)$ of the turbulent velocity components U_1,U_2,U_3 .

As Pope (Ref. 1) pointed out that, with the PDF $f_U(\boldsymbol{V};\boldsymbol{x},t)$, we can define various one-point statistical properties of the random velocity $U_i(\boldsymbol{x},t)$, for example, the mean velocity (or the first moment) $\langle U_i \rangle$:

$$\langle U_i \rangle = \int V_i \, f_U(\boldsymbol{V};\boldsymbol{x},t)\, d\boldsymbol{V} \tag{3}$$

All other higher order moments at any single point of $\boldsymbol{x},t$ (also referred as one point moments or one point correlations) can also be defined:

$$\begin{aligned} \langle U_i U_j \rangle &= \int V_i V_j \, f_U(\boldsymbol{V};\boldsymbol{x},t)\, d\boldsymbol{V} \\ \langle U_i U_j U_k \rangle &= \int V_i V_j V_k \, f_U(\boldsymbol{V};\boldsymbol{x},t)\, d\boldsymbol{V} \\ &\cdots\cdots\cdots \end{aligned} \tag{4}$$

In particular, the Reynolds stresses $\langle u_i u_j \rangle$ defined by the Reynolds decomposition $u_i = U_i - \langle U_i \rangle$ are fully defined by $f_U(\boldsymbol{V};\boldsymbol{x},t)$:

$$\langle u_i u_j \rangle = \left\langle \left(U_i - \langle U_i \rangle\right)\left(U_j - \langle U_j \rangle\right) \right\rangle = \left\langle U_i U_j - U_i \langle U_j \rangle - U_j \langle U_i \rangle + \langle U_i \rangle \langle U_j \rangle \right\rangle = \langle U_i U_j \rangle - \langle U_i \rangle \langle U_j \rangle \tag{5}$$

Equation (5) indicates that the turbulent kinetic energy $k = \langle u_i u_i \rangle / 2$ is fully defined by the velocity PDF $f_U(\boldsymbol{V};\boldsymbol{x},t)$.

2.2 PDF of Turbulent Species $f_\Phi(\psi;\boldsymbol{x},t)$

Turbulent scalar variables, for example, the species $\Phi_i(\boldsymbol{x},t), \quad i = 1,2,\cdots n$, are random variables. The PDF of species is denoted as $f_\Phi(\psi;\boldsymbol{x},t)$, where $\psi \equiv \psi_i$ is the n-dimensional sample space coordinates of the speciesΦ_i. Therefore, $f_\Phi(\psi;\boldsymbol{x},t)$ is a joint scalar PDF of multi species. Analogous to the turbulent velocity, the one-point statistical properties of the turbulent species Φ_i are fully defined by the PDF $f_\Phi(\psi;\boldsymbol{x},t)$. For example, the mean is written as

$$\langle \Phi_i \rangle = \int \psi_i \, f_\Phi(\psi;\boldsymbol{x},t)\, d\psi, \qquad i = 1, 2, \cdots, n \tag{6}$$

And the higher order moment as:

$$\begin{aligned} \langle \Phi_i^2 \rangle &= \int \psi_i^2 \, f_\Phi(\psi;\boldsymbol{x},t)\, d\psi \\ \langle \Phi_i^3 \rangle &= \int \psi_i^3 \, f_\Phi(\psi;\boldsymbol{x},t)\, d\psi \\ \langle \Phi_1 \Phi_2 \cdots \Phi_n \rangle &= \int \psi_1 \psi_2 \cdots \psi_n \, f_\Phi(\psi;\boldsymbol{x},t)\, d\psi \\ &\cdots\cdots\cdots \end{aligned} \tag{7}$$

In particular, the i^{th} species fluctuating intensity $\langle \phi_i^2 \rangle$ defined by the Reynolds decomposition $\phi_i = \Phi_i - \langle \Phi_i \rangle$ is fully defined by $f_\Phi(\psi;\boldsymbol{x},t)$,

$$\langle \phi_i^2 \rangle = \left\langle \left(\Phi_i - \langle \Phi_i \rangle\right)^2 \right\rangle = \langle \Phi_i^2 \rangle - \langle \Phi_i \rangle \langle \Phi_i \rangle \tag{8}$$

2.3 Other Turbulent Quantities and Functions of Turbulent Variables

There are several other turbulent quantities, for example, the pressure P, the chemical reaction source $S(\Phi_i)$, the pressure gradient $\partial P/\partial x_i$, the velocity gradient ∇U_i, and the higher order derivatives such as $\nabla^2 U_i$, $\nabla^2 \Phi_i$. They may be viewed as other separate random (scalar or vector) variables, in addition to the turbulent velocity U_i and the species Φ_i. We will see later that these "random variables" often appear as a "conditional mean" in the traditional PDF equations.

There are two types of quantities: one is the analytical function of the turbulent variables such as $S(\Phi_i) = \Phi_1^{\alpha}\Phi_2^{\beta}\cdots$, and the other is the derivatives of the turbulent variables such as $\nabla^2\Phi_i$. The quantities $S(\Phi_i)$ and $\nabla^2\Phi_i$ are both random because Φ_i is random. From the probability theory the statistical properties of $S(\Phi_i)$ and Φ_i can be determined by the same PDF $f_\Phi(\psi; \boldsymbol{x}, t)$. However, the statistical properties of $\nabla^2\Phi_i$ is not that straightforward.

2.3.1 Statistical Mean of Analytical Function of Turbulent Variable $S(\Phi_i)$

The statistical mean of $S(\Phi_i)$ is defined as

$$\left\langle S(\Phi_i)\right\rangle = \int S(\psi_i)\, f_\Phi(\psi; \boldsymbol{x}, t)\, d\boldsymbol{\psi} \tag{9}$$

where $S(\psi_i)$ is the functional form in the sample space $\boldsymbol{\psi}$ for $S(\Phi_i)$. The function S( ) is the assumed analytical function.

2.3.2 Statistical Mean of Derivatives of Turbulent Variable $\partial U_i/\partial x_j$ and $\partial^2 U_i/\partial x_j \partial x_j$

There are at least two ways to take means on the derivatives of velocity. Let us first use the commutation rule (Section 3.1) to express the following means:

$$\begin{aligned}
\left\langle \nabla U_i\right\rangle &= \nabla\left\langle U_i\right\rangle = \nabla\int V_i\, f_U(\boldsymbol{V}; \boldsymbol{x}, t)\, d\boldsymbol{V} = \int V_i \frac{\partial f_U(\boldsymbol{V}; \boldsymbol{x}, t)}{\partial x_j} d\boldsymbol{V} \\
\left\langle \nabla^2 U_i\right\rangle &= \int V_i \frac{\partial^2 f_U(\boldsymbol{V}; \boldsymbol{x}, t)}{\partial x_j \partial x_j} d\boldsymbol{V}
\end{aligned} \tag{10}$$

Hence, the mean of derivatives can be determined by the derivatives of the PDF of turbulent variable. Equation (10) can be further expressed as

$$\begin{aligned}
\left\langle \nabla U_i\right\rangle &= \int\left(\frac{V_i}{f_U}\frac{\partial f_U}{\partial x_j}\right) f_U(\boldsymbol{V}; \boldsymbol{x}, t) d\boldsymbol{V} \\
\left\langle \nabla^2 U_i\right\rangle &= \int\left(\frac{V_i}{f_U}\frac{\partial^2 f_U}{\partial x_j \partial x_j}\right) f_U(\boldsymbol{V}; \boldsymbol{x}, t) d\boldsymbol{V}
\end{aligned}$$

or

$$\begin{aligned}
\left\langle \nabla U_i\right\rangle &= \int D_j(V_i)\, f_U(\boldsymbol{V}; \boldsymbol{x}, t)\, d\boldsymbol{V} \\
\left\langle \nabla^2 U_i\right\rangle &= \int L(V_i)\, f_U(\boldsymbol{V}; \boldsymbol{x}, t)\, d\boldsymbol{V}
\end{aligned} \tag{11}$$

where $D_j(V_i)$ and $L(V_i)$ are defined as

$$D_j(V_i) = \frac{V_i}{f_U(\boldsymbol{V};\boldsymbol{x},t)} \frac{\partial f_U(\boldsymbol{V};\boldsymbol{x},t)}{\partial x_j}$$
$$L(V_i) = \frac{V_i}{f_U(\boldsymbol{V};\boldsymbol{x},t)} \frac{\partial^2 f_U(\boldsymbol{V};\boldsymbol{x},t)}{\partial x_j \partial x_j} \tag{12}$$

Analogy to Equation (9), we may view $D_j(V_i)$ and $L(V_i)$ as the functional forms of ∇U_i and $\nabla^2 U_i$ in the sample space $\boldsymbol{V}$.

Another way to take mean on the derivatives of velocity is to view them as some different random variables from the velocity; hence it will involve the joint PDF or the condition means of the velocity derivatives. This will be described in the next Section, where the relationships between the conditional means and the functions $D_j(V_i)$, $L(V_i)$ will be revealed.

2.4 Joint PDF

2.4.1 Joint PDF and Marginal PDF

The Navier-Stokes equations contain several random variables, for example, the velocity U_i, the pressure P (or the pressure gradient ∇P) and the molecular diffusion $\nu\nabla^2 U_i$. The scalar transport equations contain the velocity U_i, the species Φ_i and its molecular diffusion $\Gamma\nabla^2\Phi_i$. Hence a joint PDF for the joint variables of U_i, Φ_i, P, $\nabla^2 U_i \equiv L^{U_i}$, $\nabla^2\Phi_i \equiv L^{\Phi_i}, \cdots$, i.e. $f_{U,\Phi,P,L^U,L^\Phi}(\boldsymbol{V},\psi,p,\boldsymbol{l^U},\boldsymbol{l^\Phi};\boldsymbol{x},t)$, may be needed in the analysis together with the marginal PDF, such as $f_U(\boldsymbol{V};\boldsymbol{x},t)$, $f_\Phi(\psi;\boldsymbol{x},t)$, and the joint PDF of $f_{U,\Phi}(\boldsymbol{V},\psi;\boldsymbol{x},t)$. The arguments $p,\boldsymbol{l^U},\boldsymbol{l^\Phi}$ are the sample space variables of P, $\nabla^2 U_i$ and $\nabla^2\Phi_i$, respectively.

By definition, PDF must satisfy the normalization condition:

$$\int\!\!\int\!\!\int\!\!\int\!\!\int f_{U,\Phi,P,L^U,L^\Phi}(\boldsymbol{V},\psi,p,\boldsymbol{l^U},\boldsymbol{l^\Phi};\boldsymbol{x},t)d\boldsymbol{V}d\psi dp\, d\boldsymbol{l^U} d\boldsymbol{l^\Phi} = 1 \tag{13}$$

The relationship between the joint PDF $f_{U,\Phi,P,L^U,L^\Phi}(\boldsymbol{V},\psi,p,\boldsymbol{l^U},\boldsymbol{l^\Phi};\boldsymbol{x},t)$ and the marginal PDF $f_U(\boldsymbol{V};\boldsymbol{x},t)$, $f_\Phi(\psi;\boldsymbol{x},t)$, $f_P(p;\boldsymbol{x},t)$, $f_{L^U}(\boldsymbol{l^U};\boldsymbol{x},t)$ $f_{L^\Phi}(\boldsymbol{l^\Phi};\boldsymbol{x},t)$ are defined as

$$\begin{aligned}
f_U(\boldsymbol{V};\boldsymbol{x},t) &= \int\!\!\int\!\!\int\!\!\int f_{U,\Phi,P,L^U,L^\Phi}(\boldsymbol{V},\psi,p,\boldsymbol{l^U},\boldsymbol{l^\Phi};\boldsymbol{x},t)\, d\psi dp d\boldsymbol{l^U} d\boldsymbol{l^\Phi} \\
f_\Phi(\psi;\boldsymbol{x},t) &= \int\!\!\int\!\!\int\!\!\int f_{U,\Phi,P,L^U,L^\Phi}(\boldsymbol{V},\psi,p,\boldsymbol{l^U},\boldsymbol{l^\Phi};\boldsymbol{x},t)\, d\boldsymbol{V} dp d\boldsymbol{l^U} d\boldsymbol{l^\Phi} \\
f_P(p;\boldsymbol{x},t) &= \int\!\!\int\!\!\int\!\!\int f_{U,\Phi,P,L^U,L^\Phi}(\boldsymbol{V},\psi,p,\boldsymbol{l^U},\boldsymbol{l^\Phi};\boldsymbol{x},t)\, d\boldsymbol{V} d\psi d\boldsymbol{l^U} d\boldsymbol{l^\Phi} \\
f_{L^U}(\boldsymbol{l^U};\boldsymbol{x},t) &= \int\!\!\int\!\!\int\!\!\int f_{U,\Phi,P,L^U,L^\Phi}(\boldsymbol{V},\psi,p,\boldsymbol{l^U},\boldsymbol{l^\Phi};\boldsymbol{x},t)\, d\boldsymbol{V} d\psi dp d\boldsymbol{l^\Phi} \\
f_{L^\Phi}(\boldsymbol{l^\Phi};\boldsymbol{x},t) &= \int\!\!\int\!\!\int\!\!\int f_{U,\Phi,P,L^U,L^\Phi}(\boldsymbol{V},\psi,p,\boldsymbol{l^U},\boldsymbol{l^\Phi};\boldsymbol{x},t)\, d\boldsymbol{V} d\psi dp d\boldsymbol{l^U}
\end{aligned} \tag{14}$$

This is clearly required by the normalization condition for any type of PDF, including the marginal and joint PDF. With this basic concept, we can obtain various relationships between different joint PDF, for example, the joint PDF of U_i and Φ_i can be defined as

$$f_{U,\Phi}(\boldsymbol{V},\psi;\boldsymbol{x},t) = \int\!\!\int\!\!\int f_{U,\Phi,P,L^U,L^\Phi}(\boldsymbol{V},\psi,p,\boldsymbol{l^U},\boldsymbol{l^\Phi};\boldsymbol{x},t)\, dp d\boldsymbol{l^U} d\boldsymbol{l^\Phi} \tag{15}$$

It should be noted from Equations (13) and (14) that the statistical mean of a random variable can be equally define by either the joint PDF or its marginal PDF, for example,

$$
\begin{aligned}
\langle U_i \rangle &= \int\!\!\int\!\!\int\!\!\int\!\!\int V_i f_{U,\Phi,P,L^U,L^\Phi}(\boldsymbol{V},\psi,p,\boldsymbol{l^U},\boldsymbol{l^\Phi};\boldsymbol{x},t)d\boldsymbol{V}d\psi dp\, d\boldsymbol{l^U}\, d\boldsymbol{l^\Phi} \\
&= \int V_i \left(\int\!\!\int\!\!\int\!\!\int f_{U,\Phi,P,L^U,L^\Phi}(\boldsymbol{V},\psi,p,\boldsymbol{l^U},\boldsymbol{l^\Phi};\boldsymbol{x},t)d\psi dp\, d\boldsymbol{l^U}\, d\boldsymbol{l^\Phi} \right) d\boldsymbol{V} \\
&= \int V_i\; f_U(\boldsymbol{V};\boldsymbol{x},t)\, d\boldsymbol{V}
\end{aligned} \tag{16}
$$

$$
\begin{aligned}
\langle \Phi_i \rangle &= \int\!\!\int\!\!\int\!\!\int\!\!\int \psi_i f_{U,\Phi,P,L^U,L^\Phi}(\boldsymbol{V},\psi,p,\boldsymbol{l^U},\boldsymbol{l^\Phi};\boldsymbol{x},t)d\boldsymbol{V}d\boldsymbol{\psi} dp\, d\boldsymbol{l^U}\, d\boldsymbol{l^\Phi} \\
&= \int \psi_i \left(\int\!\!\int\!\!\int\!\!\int f_{U,\Phi,P,L^U,L^\Phi}(\boldsymbol{V},\psi,p,\boldsymbol{l^U},\boldsymbol{l^\Phi};\boldsymbol{x},t)\, d\boldsymbol{V}dp d\boldsymbol{l^U}\, d\boldsymbol{l^\Phi} \right) d\psi \\
&= \int \psi_i\; f_\Phi(\psi;\boldsymbol{x},t)\, d\psi
\end{aligned} \tag{17}
$$

$$
\begin{aligned}
\langle U_i \Phi_j \rangle &= \int\!\!\int\!\!\int\!\!\int\!\!\int V_i\, \psi_j\, f_{U,\Phi,P,L^U,L^\Phi}(\boldsymbol{V},\psi,p,\boldsymbol{l^U},\boldsymbol{l^\Phi};\boldsymbol{x},t)d\boldsymbol{V}d\psi dp\, d\boldsymbol{l^U}\, d\boldsymbol{l^\Phi} \\
&= \int\!\!\int V_i\, \psi_i \left(\int\!\!\int\!\!\int f_{U,\Phi,P,L^U,L^\Phi}(\boldsymbol{V},\psi,p,\boldsymbol{l^U},\boldsymbol{l^\Phi};\boldsymbol{x},t) dp d\boldsymbol{l^U}\, d\boldsymbol{l^\Phi} \right) d\boldsymbol{V} d\psi \\
&= \int\!\!\int V_i\, \psi_i\; f_{U,\Phi}(\boldsymbol{V},\psi;\boldsymbol{x},t)\, d\boldsymbol{V} d\psi
\end{aligned} \tag{18}
$$

Equations (16), (17) and (18) indicate that taking mean of a random variable only needs the relevant marginal PDF or the relevant joint PDF.

2.4.2 Conditional PDF and Conditional Mean

Let us examine an expression:

$$
\int V_i\; f_{U,\Phi}(\boldsymbol{V},\psi;\boldsymbol{x},t)\, d\boldsymbol{V} \tag{19}
$$

which is taking mean on the random variable U_i at a fixed ψ, i.e. $\Phi_i = \psi_i$. If we define the ratio of the joint PDF to the marginal PDF as

$$
f_{U|\Phi}(\boldsymbol{V}|\psi;\boldsymbol{x},t) = \frac{f_{U,\Phi}(\boldsymbol{V},\psi;\boldsymbol{x},t)}{f_\Phi(\psi;\boldsymbol{x},t)} \tag{20}
$$

Then the expression (19) can be written as

$$
\begin{aligned}
\int V_i\; f_{U,\Phi}(\boldsymbol{V},\psi;\boldsymbol{x},t)\, d\boldsymbol{V} &= f_\Phi(\psi;\boldsymbol{x},t)\cdot \int V_i\; f_{U|\Phi}(\boldsymbol{V}|\psi;\boldsymbol{x},t)\, dV_i \\
&= f_\Phi(\psi;\boldsymbol{x},t)\cdot \langle U_i | \boldsymbol{\psi} \rangle
\end{aligned} \tag{21}
$$

Where $\langle U_i | \psi \rangle$ is an abbreviation of $\langle U_i | \boldsymbol{\Phi} = \psi \rangle$ and is referred to as the conditional mean of U_i on the condition of $\Phi_i = \psi_i$:

$$
\langle U_i | \psi \rangle \equiv \int V_i\; f_{U|\Phi}(\boldsymbol{V}|\psi;\boldsymbol{x},t)\, d\boldsymbol{V} \tag{22}
$$

And $f_{U|\Phi}(\boldsymbol{V}|\psi;\boldsymbol{x},t)$ is referred to as the conditional PDF of U_i on the condition of $\Phi_i = \psi_i$, which satisfies the normalization condition because of the definition (20):

$$
\int f_{U|\Phi}(\boldsymbol{V}|\psi;\boldsymbol{x},t)\, d\boldsymbol{V} = 1 \tag{23}
$$

Similarly, the conditional mean of the random pressure $P(\boldsymbol{x},t)$ on the condition of $U_i = V_i$ is denoted as $\left\langle P(\boldsymbol{x},t) \middle| \boldsymbol{V} \right\rangle$ or $\left\langle P \middle| \boldsymbol{V} \right\rangle$ and the corresponding conditional PDF is denoted as $f_{\Phi,P,L^U,L^\Phi|U}(\psi, p, \boldsymbol{l^U}, \boldsymbol{l^\Phi} | \boldsymbol{V}, ; \boldsymbol{x},t)$, then we may naturally write

$$\begin{aligned} \left\langle P(\boldsymbol{x},t) \middle| \boldsymbol{V} \right\rangle &= \iiiint p \, f_{\Phi,P,L^U,L^\Phi|U}(\psi, p, \boldsymbol{l^U}, \boldsymbol{l^\Phi} | \boldsymbol{V}, ; \boldsymbol{x},t) \, d\psi \, dp d\boldsymbol{l^U} \, d\boldsymbol{l^\Phi} \\ &= \int p \, f_{P|U}(p|\boldsymbol{V} ; \boldsymbol{x},t) \, dp \end{aligned} \tag{24}$$

The above conditional PDF is defined as

$$f_{\Phi,P,L^U,L^\Phi|U}(\psi, p, \boldsymbol{l^U}, \boldsymbol{l^\Phi} | \boldsymbol{V}, ; \boldsymbol{x},t) = \frac{f_{U,\Phi,P,L^U,L^\Phi}(\boldsymbol{V}, \psi, p, \boldsymbol{l^U}, \boldsymbol{l^\Phi} ; \boldsymbol{x},t)}{f_U(\boldsymbol{V} ; \boldsymbol{x},t)} \tag{25}$$

or

$$f_{P|U}(p|\boldsymbol{V} ; \boldsymbol{x},t) = \frac{f_{U,P}(\boldsymbol{V}, p ; \boldsymbol{x},t)}{f_U(\boldsymbol{V} ; \boldsymbol{x},t)} \tag{26}$$

In Equations (24) and (25), the sample space variables $\psi, \boldsymbol{l^U}, \boldsymbol{l^\Phi}$ are irrelevant.

2.4.3 Relationship Between Unconditional Mean and Conditional Mean

It should be noted from Equation (24) that a conditional mean is a function of the sample space variable that has been excluded from the process of conditional mean (e.g., V_i in this case). Obviously, $\left\langle P \middle| \boldsymbol{V} \right\rangle$ is a function of sample space variable V_i, and taking 'mean' on $\left\langle P \middle| \boldsymbol{V} \right\rangle$ over the sample space V_i will lead to its unconditional mean (or just mean) pressure $\left\langle P \right\rangle$, which is a function of x_i, t .:

$$\begin{aligned} \int \left\langle P \middle| \boldsymbol{V} \right\rangle f_U(\boldsymbol{V} ; \boldsymbol{x},t) \, d\boldsymbol{V} &= \int \left(\int p \, f_{P|U}(p|\boldsymbol{V} ; \boldsymbol{x},t) \, dp \right) f_U(\boldsymbol{V} ; \boldsymbol{x},t) \, dV_i \\ &= \iint p \, f_{U,P}(\boldsymbol{V}, p ; \boldsymbol{x},t) \, d\boldsymbol{V} dp \\ &= \left\langle P \right\rangle \end{aligned}$$

Or vice versa,

$$\left\langle P \right\rangle = \iint p \, f_{U,P}(\boldsymbol{V}, p; \boldsymbol{x},t) \, d\boldsymbol{V} dp = \int f_U(\boldsymbol{V}; \boldsymbol{x},t) \left\langle P(\boldsymbol{x},t) \middle| \boldsymbol{V} \right\rangle d\boldsymbol{V} \tag{27}$$

Equation (27) is a general formula for two or more different random variables (P and U_i in this case) involved in the conditional mean of one random variable (P in this case).

Now, following Equation (27), we may straightforwardly express the means of the derivatives of turbulent velocity ∇U_i, $\nabla^2 U_i$ as

$$\begin{aligned} \left\langle \nabla U_i \right\rangle &= \int f_U(\boldsymbol{V}; \boldsymbol{x},t) \left\langle \nabla U_i \middle| \boldsymbol{V} \right\rangle d\boldsymbol{V} \\ \left\langle \nabla^2 U_i \right\rangle &= \int f_U(\boldsymbol{V}; \boldsymbol{x},t) \left\langle \nabla^2 U_i \middle| \boldsymbol{V} \right\rangle d\boldsymbol{V} \end{aligned} \tag{28}$$

Comparing Equation (28) with Equation (11), a sufficient (but not necessary) condition for this identity is

$$
\begin{aligned}
\left\langle \nabla U_i \middle| \boldsymbol{V} \right\rangle &= D_j(V_i) = \frac{V_i}{f_U}\frac{\partial f_U}{\partial x_j} \\
\left\langle \nabla^2 U_i \middle| \boldsymbol{V} \right\rangle &= L(V_i) = \frac{V_i\ \nabla^2 f_U}{f_U}
\end{aligned}
\tag{29}
$$

Equation (29) indicates the relationship between the conditional means and functions $D_j(V_i)$, $L(V_i)$. It is noted here that these equations can also be derived by using the fine grained PDF through similar sufficient condition (see Appendix A: Equations (100) and (103)).

For the mean of pressure gradient $\left\langle \partial P(x_i,t)/\partial x_i \right\rangle$, following Equation (27), we may write

$$
\left\langle \frac{\partial P}{\partial x_i} \right\rangle = \int f_U(\boldsymbol{V};\boldsymbol{x},t) \left\langle \frac{\partial P(x_i,t)}{\partial x_i} \middle| \boldsymbol{V} \right\rangle d\boldsymbol{V} \tag{30}
$$

In the past, the conditional mean of the pressure gradient in Equation (30) has been considered as an unknown quantity even if $P = P\,(U)$ was assumed. This conditional mean, like the other conditional mean $\left\langle \nabla^2 U_i \middle| \boldsymbol{V} \right\rangle$, is actually carried by the traditional velocity PDF equation and is modeled empirically. Now, if we use the rule of commutation and take the mean on the pressure gradient (assuming that $P(\boldsymbol{x},t) = P(U(\boldsymbol{x},t))$, or $P(\boldsymbol{x},t) = P(U(\boldsymbol{x},t),\, \boldsymbol{x},t)$), we may write

$$
\begin{aligned}
\left\langle \frac{\partial P}{\partial x_i} \right\rangle &= \frac{\partial}{\partial x_i}\left\langle P \right\rangle = \frac{\partial}{\partial x_i}\int P(V)\ f_U(\boldsymbol{V};\boldsymbol{x},t)\ d\boldsymbol{V} \\
&= \int \frac{\partial}{\partial x_i}\left(P(V)\, f_U(\boldsymbol{V};\boldsymbol{x},t)\right) d\boldsymbol{V} \\
&= \int \left(\frac{1}{f_U}\frac{\partial P(V)\, f_U}{\partial x_i} \right) f_U(\boldsymbol{V};\boldsymbol{x},t)\ d\boldsymbol{V} \\
&= \int P_i^g(V)\ f_U(\boldsymbol{V};\boldsymbol{x},t)\ d\boldsymbol{V}
\end{aligned}
\tag{31}
$$

Here, $P(V)$ is dependent on $\boldsymbol{x},t$ in general and $P_i^g(V)$ is defined as

$$
P_i^g(V) = \frac{1}{f_U}\frac{\partial\left[P(V)\, f_U \right]}{\partial x_i} \tag{32}
$$

Comparing Equations (30) and (31), and using a similar argument that leads to Equation (29), we obtain a relationship between the conditional mean and the function $P_i^g(V)$:

$$
\left\langle \frac{\partial P(x_i,t)}{\partial x_i} \middle| \boldsymbol{V} \right\rangle = P_i^g(V) = \frac{1}{f_U}\frac{\partial\left[P(V)\, f_U \right]}{\partial x_i} \tag{33}
$$

It is noted here that this equation can also be derived by using the fine grained PDF through the similar sufficient condition (see Appendix A: Eq. (104))

Now let us look at the mean of the product $U_i \cdot \Phi_n$, i.e. $\left\langle U_i\, \Phi_n \right\rangle$. By definition we may write

$$\begin{aligned}\left\langle U_i\,\Phi_n\right\rangle &= \int \psi_n \left(\int V_i\, f_{U,\Phi}(\boldsymbol{V},\boldsymbol{\psi};\,\boldsymbol{x},t)d\boldsymbol{V}\right)d\boldsymbol{\psi} \\ &= \int \psi_n\ f_{\Phi}(\boldsymbol{\psi};\,\boldsymbol{x},t)\left\langle U_i\middle|\boldsymbol{\psi}\right\rangle d\boldsymbol{\psi}\end{aligned} \tag{34}$$

or

$$\begin{aligned}\left\langle U_i\,\Phi_n\right\rangle &= \int V_i \left(\int \psi_n\, f_{U,\Phi}(\boldsymbol{V},\boldsymbol{\psi};\,\boldsymbol{x},t)d\boldsymbol{\psi}\right)d\boldsymbol{V} \\ &= \int V_i\ f_U(\boldsymbol{V};\,\boldsymbol{x},t)\left\langle \Phi_n\middle|\boldsymbol{V}\right\rangle d\boldsymbol{V}\end{aligned} \tag{35}$$

Equations (34) and (35) illustrate that, when taking joint mean, the joint PDF must be used to avoid the appearance of the conditional mean. The conditional mean $\left\langle U_i\middle|\boldsymbol{\psi}\right\rangle$ is also carried by the current traditional species PDF equation.

Finally, let us examine the mean and the conditional mean of a function of the variables Φ_i, say $S(\Phi_1\Phi_2\cdots\Phi_n)$, on the condition of $\boldsymbol{\Phi} = \boldsymbol{\psi}$. Let us first view $S(\Phi_1\Phi_2\cdots\Phi_n)$ as a separate random variable with the sample space variable s which is independent of $\boldsymbol{\psi}$, then, following Equation (27), we write the mean as

$$\left\langle S(\Phi_1\Phi_2\cdots\Phi_n)\right\rangle = \int f_{\Phi}(\boldsymbol{\psi};\,\boldsymbol{x},t)\left\langle S(\Phi_1\Phi_2\cdots\Phi_n)\middle|\boldsymbol{\psi}\right\rangle d\boldsymbol{\psi} \tag{36}$$

The conditional mean in (36) is

$$\begin{aligned}\left\langle S(\Phi_1\Phi_2\cdots\Phi_n)\middle|\boldsymbol{\psi}\right\rangle &= \int S(\psi_1\psi_2\cdots\psi_n)\ f_{S|\Phi}(s|\boldsymbol{\psi};\,\boldsymbol{x},t)\,ds \\ &= S(\psi_1\psi_2\cdots\psi_n)\int f_{S|\Phi}(s|\boldsymbol{\psi};\,\boldsymbol{x},t)\,ds \\ &= S(\psi_1\psi_2\cdots\psi_n)\end{aligned} \tag{37}$$

Then Equation (36) will end up an expression that is just the definition of its mean:

$$\left\langle S(\Phi_1\Phi_2\cdots\Phi_n\right\rangle = \int S(\psi_1\psi_2\cdots\psi_n)\,f_{\Phi}(\boldsymbol{\psi};\,\boldsymbol{x},t)\,d\boldsymbol{\psi} \tag{38}$$

This term is related to the chemical reaction rate in the traditional species PDF equation, which is in a closed form. Also note that the reason for the conditional mean of $S(\Phi_1\Phi_2\cdots\Phi_n)$ in Equation (36) becoming free from the constraint is that $S(\Phi_1\Phi_2\cdots\Phi_n)$ is a known function of Φ_i without involving spatial differentiation.

2.4.4 Summary

2.4.4.1 Formulations With the Conditional Mean

$$\left\langle\nabla^2 U_i\right\rangle = \int f_U(\boldsymbol{V};\,\boldsymbol{x},t)\left\langle\nabla^2 U_i\middle|\boldsymbol{V}\right\rangle d\boldsymbol{V} \tag{39}$$

$$\left\langle\nabla P\right\rangle = \int f_U(\boldsymbol{V};\,\boldsymbol{x},t)\left\langle\nabla P\middle|\boldsymbol{V}\right\rangle d\boldsymbol{V} \tag{40}$$

$$\left\langle\nabla^2 \Phi_i\right\rangle = \int f_{\Phi}(\boldsymbol{\psi};\,\boldsymbol{x},t)\left\langle\nabla^2 \Phi_i\middle|\boldsymbol{\psi}\right\rangle d\boldsymbol{\psi} \tag{41}$$

$$\left\langle S_i(\Phi_1\Phi_2\cdots\Phi_n)\right\rangle = \int f_\Phi(\psi;\boldsymbol{x},t)\left\langle S_i\middle|\psi\right\rangle d\psi \quad (42)$$

$$\left\langle U_i\,\Phi_n\right\rangle = \int \psi_n\, f_\Phi(\psi;\boldsymbol{x},t)\left\langle U_i\middle|\psi\right\rangle d\psi \tag{43}$$

The conditional means (except the one in Eq. (42)) are all considered as unknowns in the traditional PDF equations.

2.4.4.2 Formulations Without the Conditional Mean

$$\left\langle \nabla^2 U_i\right\rangle = \int V_i\,\nabla^2 f_U(\boldsymbol{V};\boldsymbol{x},t)\,d\boldsymbol{V}$$

or (44)

$$\left\langle \nabla^2 U_i\right\rangle = \int L(V_i)\,f_U(\boldsymbol{V};\boldsymbol{x},t)\,d\boldsymbol{V}, \qquad L(V_i)=\frac{V_i\,\nabla^2 f_U}{f_U}$$

$$\left\langle \frac{\partial P}{\partial x_i}\right\rangle = \int \frac{\partial}{\partial x_i}\left[P(V)\,f_U(\boldsymbol{V};\boldsymbol{x},t)\right]d\boldsymbol{V}$$

or (45)

$$\left\langle \frac{\partial P}{\partial x_i}\right\rangle = \int P_i^g(V)\,f_U(\boldsymbol{V};\boldsymbol{x},t)\,d\boldsymbol{V}, \qquad P_i^g(V)=\frac{1}{f_U}\frac{\partial\left[P(V)\,f_U\right]}{\partial x_i}$$

$$\left\langle \nabla^2\Phi_i\right\rangle = \int \psi_i\,\nabla^2 f_\Phi(\psi;\boldsymbol{x},t)\,d\psi$$

or (46)

$$\left\langle \nabla^2\Phi_i\right\rangle = \int L(\psi_i)\,f_\Phi(\psi;\boldsymbol{x},t)\,d\psi, \qquad L(\psi_i)=\frac{\psi_i\,\nabla^2 f_\Phi}{f_\Phi}$$

$$\left\langle S_i(\Phi_1\Phi_2\cdots\Phi_n)\right\rangle = \int f_\Phi(\psi;\boldsymbol{x},t)\,S_i(\psi_1\psi_2\cdots\psi_n)\,d\psi \tag{47}$$

$$\left\langle U_i\,\Phi_n\right\rangle = \int\int V_i\,\psi_n\,f_{U,\Phi}(\boldsymbol{V},\psi;\boldsymbol{x},t)\,d\boldsymbol{V}\,d\psi \quad (48)$$

These equations are exact and have no unknowns other than the PDFs f_U, f_Φ and $f_{U,\Phi}$. The functions $L(V_i)$, $L(\psi_i)$ and $P_i^g(V)$ are all well defined by the corresponding PDF, and the function $P(V)$ is assumed as known and will be defined later (Section 3.4, Equation (68)).

3.0 Transport Equation for Turbulent Velocity PDF $f_U(\boldsymbol{V};\boldsymbol{x},t)$

3.1 Mean and Differentiation Commutation

It is important to note the commutation property of taking mean and differentiation, that is

$$\left\langle \frac{\partial}{\partial t}\right\rangle = \frac{\partial\langle\ \rangle}{\partial t}, \qquad \left\langle \frac{\partial}{\partial x_i}\right\rangle = \frac{\partial\langle\ \rangle}{\partial x_i}, \qquad \left\langle \frac{\partial^2}{\partial x_i\partial x_i}\right\rangle = \frac{\partial^2\langle\ \rangle}{\partial x_i\partial x_i}, \tag{49}$$

These commutation properties have been shown in several text books, for example by Pope (Ref. 1), Tennekes and Lumley (Ref. 2). For example,

$$\left\langle \frac{\partial \boldsymbol{U}(\boldsymbol{x},t)}{\partial x_i} \right\rangle = \left\langle \lim_{\Delta x_i \to 0} \frac{\boldsymbol{U}(\boldsymbol{x}+\Delta x_i,t) - \boldsymbol{U}(\boldsymbol{x},t)}{\Delta x_i} \right\rangle = \lim_{\Delta x_i \to 0} \frac{\langle \boldsymbol{U}(\boldsymbol{x}+\Delta x_i,t)\rangle - \langle \boldsymbol{U}(\boldsymbol{x},t)\rangle}{\Delta x_i} = \frac{\partial \langle \boldsymbol{U}(\boldsymbol{x},t)\rangle}{\partial x_i} \tag{50}$$

where $\boldsymbol{U} = (U_1, U_2, U_3)$.

3.2 Taking Mean on Navier-Stokes Equations

Apply the mean operation on the Navier-Stokes equations for incompressible flow, i.e.

$$\left\langle \frac{\partial U_i}{\partial t} + \frac{\partial U_i U_j}{\partial x_j} = -\frac{1}{\rho}\frac{\partial P}{\partial x_i} + \nu \nabla^2 U_i \right\rangle. \tag{51}$$

Using the commutation rule, Equation (49), each term in Equation (51) can be expressed as follows,

$$\begin{aligned} \left\langle \frac{\partial U_i}{\partial t} \right\rangle &= \frac{\partial \langle U_i \rangle}{\partial t} = \frac{\partial}{\partial t}\int V_i\, f_U(\boldsymbol{V};\boldsymbol{x},t)\, d\boldsymbol{V} \\ &= \int V_i \left[\frac{\partial}{\partial t} f_U(\boldsymbol{V};\boldsymbol{x},t)\right] d\boldsymbol{V} \qquad \text{Note, } V_i \text{ is independent of } x_i \text{ and } t \end{aligned} \tag{52}$$

Similarly,

$$\begin{aligned} \left\langle \frac{\partial U_i U_j}{\partial x_j} \right\rangle &= \frac{\partial}{\partial x_j}\int V_i\, V_j\, f_U(\boldsymbol{V};\boldsymbol{x},t)\, d\boldsymbol{V} \\ &= \int V_i \left[V_j \frac{\partial}{\partial x_j} f_U(\boldsymbol{V};\boldsymbol{x},t)\right] d\boldsymbol{V} \end{aligned} \tag{53}$$

Taking mean on the pressure gradient term can proceed in two different ways. One is with the conditional mean, i.e., via Equation (40):

$$\begin{aligned} \left\langle -\frac{1}{\rho}\frac{\partial P}{\partial x_i} \right\rangle &= \int f_U(\boldsymbol{V};\boldsymbol{x},t) \left\langle -\frac{1}{\rho}\frac{\partial P}{\partial x_i} \middle| \boldsymbol{V} \right\rangle d\boldsymbol{V} = \int f_U(\boldsymbol{V};\boldsymbol{x},t) \left\langle -\frac{1}{\rho}\frac{\partial P}{\partial x_j} \middle| \boldsymbol{V} \right\rangle \left(\frac{\partial V_i}{\partial V_j}\right) d\boldsymbol{V}_i \\ &= \int \frac{\partial}{\partial V_j}\left(V_i\, f_U(\boldsymbol{V};\boldsymbol{x},t) \left\langle -\frac{1}{\rho}\frac{\partial P}{\partial x_j} \middle| \boldsymbol{V} \right\rangle \right) d\boldsymbol{V} - \int V_i \left(\frac{\partial}{\partial V_j}\left[f_U(\boldsymbol{V};\boldsymbol{x},t) \left\langle -\frac{1}{\rho}\frac{\partial P}{\partial x_j} \middle| \boldsymbol{V} \right\rangle \right]\right) d\boldsymbol{V} \\ &= -\int V_i \left[\frac{\partial}{\partial V_j}\left(f_U(\boldsymbol{V};\boldsymbol{x},t) \left\langle -\frac{1}{\rho}\frac{\partial P}{\partial x_j} \middle| \boldsymbol{V} \right\rangle \right)\right] d\boldsymbol{V} \qquad \text{Note, } \frac{\partial V_i}{\partial V_j} \equiv \delta_{ij} \end{aligned} \tag{54}$$

Note that the following term in Equation (54) is zero (Pope (Ref. 1) or see Appendix B):

$$\int \frac{\partial}{\partial V_j}\left(V_i\, f_U(\boldsymbol{V};\boldsymbol{x},t) \left\langle -\frac{1}{\rho}\frac{\partial P}{\partial x_j} \middle| \boldsymbol{V} \right\rangle \right) dV_i = 0 \tag{55}$$

The other way without the appearance of the conditional mean is via Equation (45)

$$
\begin{aligned}
\left\langle -\frac{1}{\rho}\frac{\partial P}{\partial x_i} \right\rangle &= -\frac{1}{\rho}\int P_j^g(V)\, f_U(\boldsymbol{V};\boldsymbol{x},t)\frac{\partial V_i}{\partial V_j}\, d\boldsymbol{V} \\
&= -\frac{1}{\rho}\int \frac{\partial}{\partial V_j}\Big(V_i\, P_j^g(V)\, f_U(\boldsymbol{V};\boldsymbol{x},t)\Big) d\boldsymbol{V} + \frac{1}{\rho}\int V_i \frac{\partial}{\partial V_j}\Big(P_j^g(V)\, f_U(\boldsymbol{V};\boldsymbol{x},t)\Big)\, d\boldsymbol{V} \qquad (56) \\
&= \int V_i\left[\frac{\partial}{\partial V_j}\left(\frac{P_j^g(V)}{\rho}\, f_U(\boldsymbol{V};\boldsymbol{x},t)\right)\right] d\boldsymbol{V}
\end{aligned}
$$

Note that (see Appendix B): $-\frac{1}{\rho}\int \frac{\partial}{\partial V_j}\Big(V_i\, P_j^g(\boldsymbol{V})\, f_U(\boldsymbol{V};\boldsymbol{x},t)\Big) d\boldsymbol{V} = 0.$

Finally, taking mean on the molecular diffusion term, one way with the conditional mean is via Equation (39),

$$
\begin{aligned}
\left\langle \nu\nabla^2 U_i \right\rangle &= \int f_U(\boldsymbol{V};\boldsymbol{x},t)\left\langle \nu\nabla^2 U_i \middle| \boldsymbol{V}\right\rangle d\boldsymbol{V} = \int f_U(\boldsymbol{V};\boldsymbol{x},t)\left\langle \nu\nabla^2 U_j \middle| \boldsymbol{V}\right\rangle \frac{\partial V_i}{\partial V_j} d\boldsymbol{V} \\
&= \int \frac{\partial}{\partial V_j}\Big(V_i\, f_U(\boldsymbol{V};\boldsymbol{x},t)\left\langle \nu\nabla^2 U_j \middle| \boldsymbol{V}\right\rangle\Big) d\boldsymbol{V} - \int V_i \frac{\partial}{\partial V_j}\Big(f_U(\boldsymbol{V};\boldsymbol{x},t)\left\langle \nu\nabla^2 U_j \middle| \boldsymbol{V}\right\rangle\Big) d\boldsymbol{V} \qquad (57) \\
&= -\int V_i\left[\frac{\partial}{\partial V_j}\Big(f_U(\boldsymbol{V};\boldsymbol{x},t)\left\langle \nu\nabla^2 U_j \middle| \boldsymbol{V}\right\rangle\Big)\right] d\boldsymbol{V}
\end{aligned}
$$

Note that (see Appendix B): $\int \frac{\partial}{\partial V_j}\Big(V_i\, f_U(\boldsymbol{V};\boldsymbol{x},t)\left\langle \nu\nabla^2 U_j \middle| \boldsymbol{V}\right\rangle\Big) d\boldsymbol{V} = 0$.

The other way without the conditional mean is via Equation (44),

$$
\begin{aligned}
\left\langle \nu\nabla^2 U_i \right\rangle &= \nu\int L(V_j)\, f_U(\boldsymbol{V};\boldsymbol{x},t)\frac{\partial V_i}{\partial V_j} d\boldsymbol{V} \\
&= \nu\int \frac{\partial}{\partial V_j}\Big(V_i\, L(V_j)\, f_U(\boldsymbol{V};\boldsymbol{x},t)\Big) d\boldsymbol{V} - \nu\int V_i \frac{\partial}{\partial V_j}\Big(L(V_j)\, f_U(\boldsymbol{V};\boldsymbol{x},t)\Big) d\boldsymbol{V} \qquad (58) \\
&= -\int V_i\left[\frac{\partial}{\partial V_j}\Big(\nu\, L(V_j)\, f_U(\boldsymbol{V};\boldsymbol{x},t)\Big)\right] d\boldsymbol{V}
\end{aligned}
$$

Note that (see Appendix B): $\nu\int \frac{\partial}{\partial V_j}\Big(V_i\, L(V_j)\, f_U(\boldsymbol{V};\boldsymbol{x},t)\Big) d\boldsymbol{V} = 0.$

3.3 Traditional Velocity PDF Equation

Now substituting Equations (52), (53), (54), (57) into Equation (51) and collecting the terms factored by V_i , a sufficient but not necessary condition for satisfying the integral equation is that the factored, total integrand is zero. Thus, a transport equation for the turbulent velocity PDF $f_U(\boldsymbol{V};\boldsymbol{x},t)$ is constructed:

$$\frac{\partial f_U}{\partial t} + V_i \frac{\partial f_U}{\partial x_i} = \frac{\partial}{\partial V_i}\left(f_U \left\langle \frac{1}{\rho}\frac{\partial P}{\partial x_i}\middle| \boldsymbol{V} \right\rangle\right) - \frac{\partial}{\partial V_i}\left(f_U \left\langle \nu \nabla^2 U_i \middle| \boldsymbol{V} \right\rangle\right) \tag{59}$$

If the pressure term is decomposed into the mean and fluctuating parts, $P = \langle P \rangle + P'$

$$\left\langle \frac{1}{\rho}\frac{\partial P}{\partial x_i}\middle| \boldsymbol{V} \right\rangle = \left\langle \frac{1}{\rho}\frac{\partial\left(\langle P \rangle + P'\right)}{\partial x_i}\middle| \boldsymbol{V} \right\rangle = \frac{1}{\rho}\frac{\partial \langle P \rangle}{\partial x_i} + \left\langle \frac{1}{\rho}\frac{\partial P'}{\partial x_i}\middle| \boldsymbol{V} \right\rangle \tag{60}$$

Then Equation (59) can be written as

$$\frac{\partial f_U}{\partial t} + V_i \frac{\partial f_U}{\partial x_i} = \frac{1}{\rho}\frac{\partial \langle P \rangle}{\partial x_i}\frac{\partial f_U}{\partial V_i} - \frac{\partial}{\partial V_i}\left(f_U \left[\left\langle \nu \nabla^2 U_i \middle| \boldsymbol{V} \right\rangle - \left\langle \frac{1}{\rho}\frac{\partial P'}{\partial x_i}\middle| \boldsymbol{V} \right\rangle \right]\right) \tag{61}$$

Equation (61) is exactly the same as the traditional velocity PDF equation (Pope (Ref. 1)). The mean pressure in Equation (61) is considered as a known quantity through its Poisson equation. However, the last two terms with the conditional mean were considered as unknown and modeled empirically. Using the following identity relations (Pope (Ref. 1)):

$$f_U(\boldsymbol{V};\boldsymbol{x},t)\left\langle \frac{\partial P'}{\partial x_i}\middle| \boldsymbol{V} \right\rangle = \frac{\partial}{\partial x_i}\left(f_U(\boldsymbol{V};\boldsymbol{x},t)\left\langle P' \middle| \boldsymbol{V} \right\rangle\right) + \frac{\partial}{\partial V_j}\left(f_U(\boldsymbol{V};\boldsymbol{x},t)\left\langle P' \frac{\partial U_j}{\partial x_i}\middle| \boldsymbol{V} \right\rangle\right) \tag{62}$$

$$\frac{\partial}{\partial V_j}\left[f_U(\boldsymbol{V};\boldsymbol{x},t)\left\langle \nabla^2 U_j \middle| \boldsymbol{V} \right\rangle\right] = \frac{\partial^2}{\partial V_j \partial V_k}\left(f_U(\boldsymbol{V};\boldsymbol{x},t)\left\langle \frac{\partial U_j}{\partial x_i}\frac{\partial U_k}{\partial x_i}\middle| \boldsymbol{V} \right\rangle\right) - \nabla^2 f_U(\boldsymbol{V};\boldsymbol{x},t) \tag{63}$$

Equation (61) can be rewritten as

$$\begin{aligned} \frac{\partial f_U}{\partial t} + V_i \frac{\partial f_U}{\partial x_i} &= \nu \nabla^2 f_U + \frac{1}{\rho}\frac{\partial \langle P \rangle}{\partial x_i}\frac{\partial f_U}{\partial V_i} + \frac{\partial^2}{\partial x_i \partial V_i}\left(f_U \left\langle \frac{P'}{\rho}\middle| \boldsymbol{V} \right\rangle\right) \\ &+ \frac{1}{2}\frac{\partial^2}{\partial V_i \partial V_j}\left(f_U \left\langle \frac{P'}{\rho}\left(\frac{\partial U_j}{\partial x_i} + \frac{\partial U_i}{\partial x_j}\right)\middle| \boldsymbol{V} \right\rangle - f_U \left\langle 2\nu \frac{\partial U_i}{\partial x_k}\frac{\partial U_j}{\partial x_k}\middle| \boldsymbol{V} \right\rangle\right) \end{aligned} \tag{64}$$

Now we have three unknown terms in Equation (64) that were modeled empirically (Pope (Ref. 1)).

3.4 Conservational Velocity PDF Equation

Alternatively, collecting the terms factored by V_i from (52), (53), (56) and (58), and following the same procedure that leads to Equation (61), we obtain a closed velocity PDF transport equation:

$$\frac{\partial f_U}{\partial t} + V_j \frac{\partial f_U}{\partial x_j} = -\frac{\partial}{\partial V_j}\left(\nu L(V_j)\, f_U \right) + \frac{\partial}{\partial V_j}\left(\frac{P_j^g(V)}{\rho} f_U \right). \tag{65}$$

Here $L(V_j)$ and $P_j^g(V)$ are known functions:

$$L(V_j) = \frac{V_j \, \nabla^2 f_U}{f_U}, \qquad P_j^g(V) = \frac{1}{f_U} \frac{\partial \left[P(V) \, f_U \right]}{\partial x_j} \tag{66}$$

In order to determine $P(V)$, we first take mean on the Poisson equation

$$\left\langle \frac{1}{\rho} \nabla^2 P = -\frac{\partial^2 U_i \, U_j}{\partial x_i \partial x_j} \right\rangle, \qquad \text{or} \qquad \frac{1}{\rho} \nabla^2 \left\langle P \right\rangle = -\frac{\partial^2 \left\langle U_i \, U_j \right\rangle}{\partial x_i \partial x_j} \tag{67}$$

By the definition of the mean, we may write Equation (67) as

$$\frac{1}{\rho} \nabla^2 \int P(V) \, f_U(\boldsymbol{V}; \boldsymbol{x}, t) \, d\boldsymbol{V} = -\frac{\partial^2}{\partial x_i \partial x_j} \int V_i \, V_j \; f_U(\boldsymbol{V}; \boldsymbol{x}, t) \, d\boldsymbol{V}$$

or

$$\frac{1}{\rho} \int \nabla^2 \left(P(V) \, f_U(\boldsymbol{V}; \boldsymbol{x}, t) \right) d\boldsymbol{V} = -\int V_i \, V_j \frac{\partial^2 f_U(\boldsymbol{V}; \boldsymbol{x}, t)}{\partial x_i \partial x_j} d\boldsymbol{V}$$

By equating the integrands on both sides (again, this is a sufficient condition for satisfying the above integral equation), we obtain a model equation for $P(V)$:

$$\frac{1}{\rho} \nabla^2 \left[P(V) \, f_U \right] = -V_i \, V_j \frac{\partial^2 f_U}{\partial x_i \partial x_j} \tag{68}$$

Therefore we have constructed a velocity PDF Equation (65) that does not need extra turbulence modeling.

Using Equation (65), it is easy to show that the exact equations for the first moment and higher order moments of the Navier-Stokes equations can be deduced by multiplying the Equation (65) with V_i and $V_i \, V_j$ respectively and integrating over the velocity sample space $\boldsymbol{V}$. For example,

$$\int V_i \, V_j \left\{ \frac{\partial f_U}{\partial t} + V_k \frac{\partial f_U}{\partial x_k} = -\frac{\partial}{\partial V_k} \left(\nu \, L(V_k) \, f_U \right) + \frac{\partial}{\partial V_k} \left(\frac{P_k^g(\boldsymbol{V})}{\rho} \, f_U \right) \right\} d\boldsymbol{V}$$

The left two terms become

$$\frac{\partial \left\langle U_i U_j \right\rangle}{\partial t} + \frac{\partial \left\langle U_i U_j U_k \right\rangle}{\partial x_k},$$

and the first term on the right hand side is,

$$\begin{aligned} -\int V_i \, V_j \frac{\partial}{\partial V_k} \left(\nu \, L(V_k) \, f_U \right) d\boldsymbol{V} &= -\int \frac{\partial}{\partial V_k} \left(V_i \, V_j \nu \, L(V_k) \, f_U \right) d\boldsymbol{V} + \int \nu \, L(V_k) \, f_U \frac{\partial V_i \, V_j}{\partial V_k} d\boldsymbol{V} \\ &= \int \left(\nu \, L(V_j) V_i \, f_U + \nu \, L(V_i) V_j \, f_U \right) d\boldsymbol{V} \\ &= \nu \left\langle U_i \, \nabla^2 U_j + U_j \, \nabla^2 U_i \right\rangle \end{aligned}$$

Note that (see Appendix B): $-\int \frac{\partial}{\partial V_k}\left(V_i V_j \nu L(V_k) f_U\right) d\boldsymbol{V} = 0.$

Similarly, the second term on the right hand side is

$$\int V_i V_j \frac{\partial}{\partial V_k}\left(\frac{P_k^g(\boldsymbol{V})}{\rho} f_U\right) d\boldsymbol{V} = -\frac{1}{\rho}\left\langle U_i \frac{\partial P}{\partial x_j} + U_j \frac{\partial P}{\partial x_i}\right\rangle$$

Therefore we obtain the exact equation for the second moment $\left\langle U_i U_j \right\rangle$:

$$\frac{\partial \left\langle U_i U_j \right\rangle}{\partial t} + \frac{\partial \left\langle U_i U_j U_k \right\rangle}{\partial x_k} = -\frac{1}{\rho}\left\langle U_i \frac{\partial P}{\partial x_j} + U_j \frac{\partial P}{\partial x_i}\right\rangle + \nu \left\langle U_i \nabla^2 U_j + U_j \nabla^2 U_i \right\rangle \tag{69}$$

4.0 Transport Equation for Turbulent Species PDF $f_\Phi(\psi; \boldsymbol{x}, t)$

4.1 Taking Mean on Species Equation

Taking mean on the transport equation for species Φ_i

$$\left\langle \frac{\partial \Phi_i}{\partial t} + \frac{\partial \Phi_i U_j}{\partial x_j} = \Gamma \nabla^2 \Phi_i + S_i(\Phi_1 \Phi_2 \cdots \Phi_n) \right\rangle \tag{70}$$

The first term on the L.H.S. of (70) can be written as

$$\begin{aligned} \frac{\partial \left\langle \Phi_i \right\rangle}{\partial t} &= \frac{\partial}{\partial t}\int\int \left(\psi_i f_{U,\Phi}(\boldsymbol{V}, \psi; \boldsymbol{x}, t)\right) d\boldsymbol{V} d\psi = \int \psi_i \frac{\partial}{\partial t}\left(\int f_{U,\Phi}(\boldsymbol{V}, \psi; \boldsymbol{x}, t) d\boldsymbol{V}\right) d\psi \\ &= \int \psi_i \left[\frac{\partial}{\partial t} f_\Phi(\psi; \boldsymbol{x}, t)\right] d\psi \end{aligned} \tag{71}$$

Equation (71) involves a marginal PDF f_Φ. We can also write this term using the joint PDF $f_{U,\Phi}$:

$$\begin{aligned} \frac{\partial \left\langle \Phi_i \right\rangle}{\partial t} &= \frac{\partial}{\partial t}\int\int \left(\psi_i f_{U,\Phi}(\boldsymbol{V}, \psi; \boldsymbol{x}, t)\right) d\boldsymbol{V} d\psi \\ &= \int\int \psi_i \left[\frac{\partial}{\partial t}\left(f_{U,\Phi}(\boldsymbol{V}, \psi; \boldsymbol{x}, t)\right)\right] d\boldsymbol{V} d\psi \end{aligned} \tag{72}$$

The second term on the L.H.S. of (70) can also be formed in two ways:

$$\begin{aligned} \frac{\partial \left\langle \Phi_i U_j \right\rangle}{\partial x_j} &= \frac{\partial}{\partial x_j}\int\int \psi_i V_j f_{U,\Phi}(\boldsymbol{V}, \psi; \boldsymbol{x}, t) d\boldsymbol{V} d\psi \\ &= \int \psi_i \left[\frac{\partial}{\partial x_j} f_\Phi(\psi; \boldsymbol{x}, t) \left\langle U_j \middle| \psi \right\rangle\right] d\psi \end{aligned} \tag{73}$$

or

$$\begin{aligned}\frac{\partial\left\langle \Phi_i U_j\right\rangle}{\partial x_j} &= \frac{\partial}{\partial x_j}\int\int \psi_i V_j\, f_{U,\Phi}(\boldsymbol{V},\psi;\, \boldsymbol{x},t)\, d\boldsymbol{V} d\boldsymbol{\psi} \\ &= \int\int \psi_i \left[V_j \frac{\partial}{\partial x_j} f_{U,\Phi}(\boldsymbol{V},\psi;\, \boldsymbol{x},t)\right] d\boldsymbol{V} d\boldsymbol{\psi}\end{aligned} \tag{74}$$

The next term $\nabla^2\Phi_i$ of (70) can again be written in two different forms: Using Equation (41), we have

$$\begin{aligned}\Gamma\left\langle \nabla^2\Phi_i\right\rangle &= \Gamma\int f_\Phi(\psi;\, \boldsymbol{x},t)\left\langle \nabla^2\Phi_i \middle| \psi\right\rangle d\boldsymbol{\psi} = \Gamma\int f_\Phi(\psi;\, \boldsymbol{x},t)\left\langle \nabla^2\Phi_j \middle| \psi\right\rangle \frac{\partial\psi_i}{\partial\psi_j} d\boldsymbol{\psi} \\ &= \Gamma\int \frac{\partial}{\partial\psi_j}\left[\psi_i f_\Phi(\psi;\, \boldsymbol{x},t)\left\langle \nabla^2\Phi_j \middle| \psi\right\rangle\right] d\boldsymbol{\psi} - \Gamma\int \psi_i \frac{\partial}{\partial\psi_j}\left(f_\Phi(\psi;\, \boldsymbol{x},t)\left\langle \nabla^2\Phi_j \middle| \psi\right\rangle\right) d\boldsymbol{\psi} \\ &= -\int \psi_i \left[\frac{\partial}{\partial\psi_j}\left(f_\Phi(\psi;\, \boldsymbol{x},t)\left\langle \Gamma\nabla^2\Phi_j \middle| \psi\right\rangle\right)\right] d\boldsymbol{\psi}\end{aligned} \tag{75}$$

Note that (see Appendix B): $\int \frac{\partial}{\partial\psi_j}\left[\psi_i f_\Phi(\psi;\, \boldsymbol{x},t)\left\langle \nabla^2\Phi_j \middle| \psi\right\rangle\right] d\boldsymbol{\psi} = 0$.

Or we can straightforwardly write its mean as

$$\begin{aligned}\Gamma\left\langle \nabla^2\Phi_i\right\rangle &= \Gamma\nabla^2\left\langle \Phi_i\right\rangle = \Gamma\nabla^2\int\int \psi_i f_{U,\Phi}(\boldsymbol{V},\psi;\, \boldsymbol{x},t)\, d\boldsymbol{V} d\boldsymbol{\psi} \\ &= \int\int \psi_i \left[\Gamma\nabla^2 f_{U,\Phi}(\boldsymbol{V},\psi;\, \boldsymbol{x},t)\right] d\boldsymbol{V} d\boldsymbol{\psi} \\ &= \int\int \Gamma L(\psi_i)\, f_{U,\Phi}(\boldsymbol{V},\psi;\, \boldsymbol{x},t)\, d\boldsymbol{V} d\boldsymbol{\psi}\end{aligned} \tag{76}$$

Where $L(\psi_i)$ is defined as

$$L(\psi_i) = \frac{\psi_i \nabla^2 f_{U,\Phi}}{f_{U,\Phi}} = \frac{\psi_i \nabla^2 f_\Phi}{f_\Phi} \tag{77}$$

Equation (76) can be further manipulated as

$$\begin{aligned}\Gamma\left\langle \nabla^2\Phi_i\right\rangle &= \Gamma\int\int L(\psi_j)\, f_{U,\Phi}(\boldsymbol{V},\psi;\, \boldsymbol{x},t)\frac{\partial\psi_i}{\partial\psi_j} d\boldsymbol{V} d\boldsymbol{\psi} \\ &= \Gamma\int\int \frac{\partial}{\partial\psi_j}\left(\psi_i\, L(\psi_j)\, f_{U,\Phi}(\boldsymbol{V},\psi;\, \boldsymbol{x},t)\right) d\boldsymbol{V} d\boldsymbol{\psi} \\ &\quad -\Gamma\int\int \psi_i \frac{\partial}{\partial\psi_j}\left(L(\psi_j)\, f_{U,\Phi}(\boldsymbol{V},\psi;\, \boldsymbol{x},t))\right) d\boldsymbol{V} d\boldsymbol{\psi} \\ &= -\Gamma\int\int \psi_i \left[\frac{\partial}{\partial\psi_j}\left(L(\psi_j)\, f_{U,\Phi}(\boldsymbol{V},\psi;\, \boldsymbol{x},t)\right)\right] d\boldsymbol{V} d\boldsymbol{\psi}\end{aligned} \tag{78}$$

Note that (see Appendix B): $\Gamma\int\int \frac{\partial}{\partial\psi_j}\left(\psi_i\, L(\psi_j)\, f_{U,\Phi}(\boldsymbol{V},\psi;\, \boldsymbol{x},t)\right) d\boldsymbol{V} d\boldsymbol{\psi} = 0$.

The reacting source term is readily available via Equation (42),

$$
\begin{aligned}
\langle S_i(\Phi_1\Phi_2\cdots\Phi_n)\rangle &= \int f_\Phi(\psi;\,\boldsymbol{x},t)\,\langle S_i|\psi\rangle\,d\boldsymbol{\psi} = \int f_\Phi(\psi;\,\boldsymbol{x},t)\langle S_j|\psi\rangle\frac{\partial\psi_i}{\partial\psi_j}\,d\boldsymbol{\psi}\\
&= \int \frac{\partial}{\partial\psi_j}\Big(\psi_i f_\Phi(\psi;\,\boldsymbol{x},t)\langle S_j|\psi\rangle\Big)d\boldsymbol{\psi} - \int \psi_i\frac{\partial}{\partial\psi_j}\Big(f_\Phi(\psi;\,\boldsymbol{x},t)\langle S_j|\psi\rangle\Big)d\boldsymbol{\psi}\\
&= -\int \psi_i\left[\frac{\partial}{\partial\psi_j}\Big(f_\Phi(\psi;\,\boldsymbol{x},t)S_j(\psi_1\psi_2\cdots\psi_n)\Big)\right]d\boldsymbol{\psi}
\end{aligned} \tag{79}
$$

Note that (see Appendix B): $\int \frac{\partial}{\partial\psi_j}\Big(\psi_i f_\Phi(\psi;\,\boldsymbol{x},t)\langle S_j|\psi\rangle\Big)d\boldsymbol{\psi} = 0$.

Another expression for the reaction source term can be obtained as

$$
\begin{aligned}
\langle S_i(\Phi_1\Phi_2\cdots\Phi_n)\rangle &= \iint S_i(\psi_1\psi\cdots\psi_n)\,f_{U,\Phi}(\boldsymbol{V},\psi;\,\boldsymbol{x},t)\,d\boldsymbol{V}d\boldsymbol{\psi}\\
&= -\iint \psi_i\left[\frac{\partial}{\partial\psi_j}\Big(S_j(\psi_1\psi\cdots\psi_n)\,f_{U,\Phi}(\boldsymbol{V},\psi;\,\boldsymbol{x},t)\Big)\right]d\boldsymbol{V}d\boldsymbol{\psi}
\end{aligned} \tag{80}
$$

Note that (see Appendix B): $\iint \frac{\partial}{\partial\psi_j}\Big(\psi_i S_j(\psi_1\psi\cdots\psi_n)\,f_{U,\Phi}(\boldsymbol{V},\psi;\,\boldsymbol{x},t)\Big)d\boldsymbol{V}d\boldsymbol{\psi} = 0$

4.2 Traditional Species PDF Equation

Collecting terms factored by ψ_i from Equations (71), (73), (75) and (79), and following the procedure similar to the construction of the velocity PDF equation, we obtain the species PDF equation:

$$
\frac{\partial f_\Phi}{\partial t} + \frac{\partial}{\partial x_j}\Big(f_\Phi\,\langle U_j|\psi\rangle\Big) = -\frac{\partial}{\partial\psi_j}\Big(f_\Phi\Big(\langle\Gamma\nabla^2\Phi_j|\psi\rangle + S_j(\psi_1\psi\cdots\psi_n)\Big)\Big) \tag{81}
$$

By using Reynolds decomposition $u_i = U_i - \langle U_i\rangle$, Equation (81) becomes

$$
\frac{\partial f_\Phi}{\partial t} + \langle U_j\rangle\frac{\partial f_\Phi}{\partial x_j} + \frac{\partial}{\partial x_j}\Big(f_\Phi\,\langle u_j|\psi\rangle\Big) = -\frac{\partial}{\partial\psi_j}\Big(f_\Phi\Big(\langle\Gamma\nabla^2\Phi_j|\psi\rangle + S_j(\psi_1\psi\cdots\psi_n)\Big)\Big) \tag{82}
$$

Equation (82) is also exactly the same as the traditional species PDF equation derived by Pope (Ref. 1), which contains two conditional means from the convection term and the molecular diffusion term. These terms were considered as unknowns and were modeled empirically.

4.3 Conservational Joint Species-Velocity PDF $f_{U,\Phi}(\boldsymbol{V},\psi;\,\boldsymbol{x},t)$ Equation

Alternatively, by collecting terms factored by ψ_i from Equations (72), (74), (78), and (80) , we obtain the following equation:

$$
\frac{\partial f_{U,\Phi}}{\partial t} + V_j\frac{\partial f_{U,\Phi}}{\partial x_j} = -\frac{\partial}{\partial\psi_j}\Big(\Gamma L(\psi_j)\,f_{U,\Phi}\Big) - \frac{\partial}{\partial\psi_j}\Big(f_{U,\Phi}S_j(\psi_1\psi\cdots\psi_n)\Big) \tag{83}
$$

Equation (83) is in closed form. They can be reduced to the marginal species PDF $f_\Phi(\psi; \boldsymbol{x},t)$ equation by integrating over the velocity sample space V_i. The result is

$$\frac{\partial f_\Phi}{\partial t} + \langle U_j \rangle \frac{\partial f_\Phi}{\partial x_j} + \frac{\partial}{\partial x_j}\Big(f_\Phi \langle u_j | \psi \rangle \Big) = -\frac{\partial}{\partial \psi_j}\Big(\Gamma\, L(\psi_j)\, f_\Phi\Big) - \frac{\partial}{\partial \psi_j}\Big(f_\Phi S_j(\psi_1\psi\cdots\psi_n)\Big) \tag{84}$$

In Equation (84), there is an unavoidable conditional mean due to the convection term that involves both the velocity and the species. The conditional mean of fluctuating velocity conditioned on $\Phi_i = \psi_i$, $\langle u_j | \psi \rangle$, is unknown and must be modeled.

Now let us return to the subject of joint PDF. Equation (83) is derived from the species diffusion Equation (70), the two source terms on the right hand side represent the molecular mixing of “species” and the chemistry reaction, respectively. We also have to consider the contribution from the Navier-Stokes equations, which can be obtained in a way similar to that leads to Equation (65):

$$\frac{\partial f_{U,\Phi}}{\partial t} + V_j \frac{\partial f_{U,\Phi}}{\partial x_j} = -\frac{\partial}{\partial V_j}\Big(\nu\, L(V_j)\, f_{U,\Phi}\Big) + \frac{\partial}{\partial V_j}\left(\frac{P_j^g(\boldsymbol{V})}{\rho}\, f_{U,\Phi}\right) \tag{85}$$

The terms on the right hand side of Equation (85) represent the molecular mixing of “momentum” and the pressure source. Therefore, the joint species-velocity PDF $f_{U_i,\Phi_i}(V_i,\psi_i; x_i,t)$ equation should include all source terms on the right hand side of Equations (83) and (85), i.e.

$$\begin{aligned}\frac{\partial f_{U,\Phi}}{\partial t} + V_j \frac{\partial f_{U,\Phi}}{\partial x_j} &= -\frac{\partial}{\partial V_j}\Big(\nu\, L(V_j)\, f_{U,\Phi}\Big) + \frac{\partial}{\partial V_j}\left(\frac{P_j^g(\boldsymbol{V})}{\rho}\, f_{U,\Phi}\right) \\ &\quad -\frac{\partial}{\partial \psi_j}\Big(\Gamma\, L(\psi_j)\, f_{U,\Phi}\Big) - \frac{\partial}{\partial \psi_j}\Big(f_{U,\Phi} S_j(\psi_1\psi\cdots\psi_n)\Big)\end{aligned} \tag{86}$$

It is easy to verify that the joint PDF $f_{U,\Phi}$ Equation (86) can be reduced to the equations for the marginal velocity PDF f_U and the marginal species PDF f_Φ by integrating over the corresponding sample space, and the results are the same as the Equations (65) and (84). It is also easy to verify that Equation (86) can deduce the exact equations for the first moments $\langle U_i \rangle$, $\langle \Phi_i \rangle$ and higher order moments $\langle \Phi_i \Phi_j \rangle$, $\langle U_i \Phi_j \rangle$, etc.

The functions involved in Equation (86), i.e., $L(V_j)$, $P_j^g(\boldsymbol{V})$, $L(\psi_j)$ are all known and given by Equations (66), (68) and (77):

$$\begin{aligned} L(V_j) &= \frac{V_j\ \nabla^2 f_{U,\Phi}}{f_{U,\Phi}} = \frac{V_j\ \nabla^2 f_U}{f_U} \\ P_j^g(V) &= \frac{1}{f_{U,\Phi}}\ \frac{\partial\big[P(V)\, f_{U,\Phi}\big]}{\partial x_j} = \frac{1}{f_U}\ \frac{\partial\big[P(V)\, f_U\big]}{\partial x_j} \\ \frac{1}{\rho} P(V) &= -\frac{V_i V_j}{\nabla^2 f_{U,\Phi}}\ \frac{\partial^2 f_{U,\Phi}}{\partial x_i \partial x_j} = -\frac{V_i V_j}{\nabla^2 f_U}\ \frac{\partial^2 f_U}{\partial x_i \partial x_j} \\ L(\psi_i) &= \frac{\psi_i \nabla^2 f_{U,\Phi}}{f_{U,\Phi}} = \frac{\psi_i \nabla^2 f_\Phi}{f_\Phi} \end{aligned} \tag{87}$$

The Following two relations, which are similar to Equation (12), are also useful:

$$
\begin{aligned}
D_j(V_i) &= \frac{V_i}{f_{U,\Phi}} \frac{\partial f_{U,\Phi}}{\partial x_j} = \frac{V_i}{f_U} \frac{\partial f_U}{\partial x_j} \\
D_j(\psi_i) &= \frac{\psi_i}{f_{U,\Phi}} \frac{\partial f_{U,\Phi}}{\partial x_j} = \frac{\psi_i}{f_\Phi} \frac{\partial f_\Phi}{\partial x_j}
\end{aligned}
\tag{88}
$$

The solution of Equation (86) should be able to calculate all one-point statistics for the velocity and species, for example, $\langle U_i \rangle, \langle \Phi_i \rangle, \langle U_i U_j \rangle, \langle U_i \Phi_i \rangle, \langle \Phi_1 \Phi_2 \cdots \rangle$, etc. We can also calculate other turbulent quantities, such as $\left\langle \frac{\partial U_i}{\partial x_k} \frac{\partial U_j}{\partial x_k} \right\rangle$, $\left\langle \frac{\partial \Phi_n}{\partial x_k} \frac{\partial \Phi_n}{\partial x_k} \right\rangle$, $\langle PU_i \rangle$ and $\langle PS_{ij} \rangle$, which are related to the dissipation rate ε_{ij}, ε, ε_{Φ_n}, the pressure transport and the pressure strain correlations, etc. For example,

$$
\varepsilon_{ij} = \nu \left(\left\langle \frac{\partial U_i}{\partial x_k} \frac{\partial U_j}{\partial x_k} \right\rangle - \left\langle \frac{\partial U_i}{\partial x_k} \right\rangle \left\langle \frac{\partial U_j}{\partial x_k} \right\rangle \right)
$$

$$
\varepsilon_{\Phi_n} = \Gamma \left(\left\langle \frac{\partial \Phi_n}{\partial x_k} \frac{\partial \Phi_n}{\partial x_k} \right\rangle - \left\langle \frac{\partial \Phi_n}{\partial x_k} \right\rangle \left\langle \frac{\partial \Phi_n}{\partial x_k} \right\rangle \right)
$$

$$
\langle pu_i \rangle = \langle PU_i \rangle - \langle P \rangle \langle U_i \rangle, \quad \langle ps_{ij} \rangle = \langle PS_{ij} \rangle - \langle P \rangle \langle S_{ij} \rangle
$$

and

$$
\begin{aligned}
\left\langle \frac{\partial U_i}{\partial x_k} \frac{\partial U_j}{\partial x_k} \right\rangle &= \int\int D_k(V_i) D_k(V_j) f_{U,\Phi} \, d\mathbf{V} d\boldsymbol{\psi} = \int D_k(V_i) D_k(V_j) f_U \, d\mathbf{V} \\
\left\langle \frac{\partial \Phi_n}{\partial x_k} \frac{\partial \Phi_n}{\partial x_k} \right\rangle &= \int\int D_k(\psi_n) D_k(\psi_n) f_{U,\Phi} \, d\mathbf{V} d\boldsymbol{\psi} = \int D_k(\psi_n) D_k(\psi_n) f_\Phi \, d\boldsymbol{\psi}
\end{aligned}
\tag{89}
$$

$$
\begin{aligned}
\langle PU_i \rangle &= \int\int P(V) V_i f_{U,\Phi} \, d\mathbf{V} d\boldsymbol{\psi} = \int P(V) V_i f_U \, d\mathbf{V} \\
\langle PS_{ij} \rangle &= \frac{1}{2} \int\int \left(P(V) \left(D_j(V_i) + D_i(V_j) \right) f_{U,\Phi} \right) d\mathbf{V} d\boldsymbol{\psi} = \frac{1}{2} \int \left(P(V) \left(D_j(V_i) + D_i(V_j) \right) f_U \right) d\mathbf{V}
\end{aligned}
\tag{90}
$$

5.0 Concluding Remarks

We have constructed a set of conservational PDF equations directly from the Navier-Stokes equations and the species diffusion equations through the use of some sufficient but not necessary conditions. Therefore, in theory, they are neither general nor unique. However, all these PDF equations are in closed form. They are able to deduce the exact transport equations for the first moment and all higher order moments. This feature has not been observed from any other existing modeled PDF equations. For example, the modeled traditional PDF equations can deduce the first moment equation correctly, but not for the higher order moments.

In this study, we have also defined a few functions, for example, $D_j(V_i)$, $L(V_i)$, $D_j(\Phi_i)$, $L(\Phi_i)$ and $P_i^g(V)$, they may be viewed as the models for the conditional means of ∇U_i, $\nabla^2 U_i$, $\nabla \Phi_i$, $\nabla^2 \Phi_i$ and ∇P. These functions may be used to calculate other turbulent quantities of interest.

Future work includes further testing of the present conservational PDF equations for their application in the area of CFD and the development of conservational filtered density function (FDF) equations for compressible turbulent flows.

Appendix A.—Fine Grained PDF, Velocity and Species PDF Equations

A.1 Transport Equation for Fine Grained PDF $f'(\boldsymbol{V};\boldsymbol{x},t)$

According to Pope (Ref. 1), the fine grained PDF $f'(\boldsymbol{V};\boldsymbol{x},t)$ is defined as

$$f'(\boldsymbol{V};\boldsymbol{x},t)=\delta\left(\boldsymbol{U}(\boldsymbol{x},t)-\boldsymbol{V}\right) \tag{91}$$

Taking the following operations,

$$\begin{aligned}\frac{\partial f'}{\partial t}&=\frac{\partial f'}{\partial U_i}\frac{\partial U_i}{\partial t}=-\frac{\partial f'}{\partial V_i}\frac{\partial U_i}{\partial t}=-\frac{\partial}{\partial V_i}\left(f'\frac{\partial U_i}{\partial t}\right)\\ \frac{\partial f'}{\partial x_j}&=\frac{\partial f'}{\partial U_i}\frac{\partial U_i}{\partial x_j}=-\frac{\partial f'}{\partial V_i}\frac{\partial U_i}{\partial x_j}=-\frac{\partial}{\partial V_i}\left(f'\frac{\partial U_i}{\partial x_j}\right)\end{aligned} \tag{92}$$

We may form an identity equation for the fine grained PDF:

$$\frac{\partial f'}{\partial t}+U_j\frac{\partial f'}{\partial x_j}=-\frac{\partial}{\partial V_i}\left\{f'\left(\frac{\partial U_i}{\partial t}+U_j\frac{\partial U_i}{\partial x_j}\right)\right\} \tag{93}$$

Inserting the Navier-Stokes equation into Equation (93), we obtain a transport equation for the fine grained PDF:

$$\frac{\partial f'}{\partial t}+U_j\frac{\partial f'}{\partial x_j}=-\frac{\partial}{\partial V_i}\left\{f'\left(-\frac{1}{\rho}\frac{\partial P}{\partial x_i}+\nu\frac{\partial^2 U_i}{\partial x_j\partial x_j}\right)\right\} \tag{94}$$

A.2 Transport Equation for Velocity PDF $f_U(\boldsymbol{V};\boldsymbol{x},t)$

Now, taking mean on Equation (94) we will obtain a transport equation for the velocity PDF. First taking mean on the left hand side of (94),

$$\begin{aligned}\left\langle\frac{\partial f'}{\partial t}+U_j\frac{\partial f'}{\partial x_j}\right\rangle&=\frac{\partial\langle f'\rangle}{\partial t}+\frac{\partial\langle f'U_j\rangle}{\partial x_j}\\ &=\frac{\partial}{\partial t}\int\delta(\boldsymbol{V}'-\boldsymbol{V})\,f_U(\boldsymbol{V}';\boldsymbol{x},t)\,d\boldsymbol{V}'+\frac{\partial}{\partial x_j}\int\delta(\boldsymbol{V}'-\boldsymbol{V})V_j'\,f_U(\boldsymbol{V}';\boldsymbol{x},t)\,d\boldsymbol{V}'\\ &=\frac{\partial f_U(\boldsymbol{V};\boldsymbol{x},t)}{\partial t}+V_j\frac{\partial f_U(\boldsymbol{V};\boldsymbol{x},t)}{\partial x_j}\end{aligned} \tag{95}$$

To explain the way of taking mean on the right hand side of (94), let us first take the mean on $f'\,\partial U_i/\partial x_j$, i.e.

$$\left\langle f' \frac{\partial U_i}{\partial x_j} \right\rangle = \lim_{\Delta x_j \to 0} \left\langle \delta\big(\boldsymbol{U}(\boldsymbol{x},t) - \boldsymbol{V}\big) \frac{U_i(\boldsymbol{x}+\Delta x_j,t) - U_i(\boldsymbol{x},t)}{\Delta x_j} \right\rangle$$
$$= \lim_{\Delta x_j \to 0} \left\langle \frac{\delta\big(\boldsymbol{U}(\boldsymbol{x},t) - \boldsymbol{V}\big) U_i(\boldsymbol{x}+\Delta x_j,t) - \delta\big(\boldsymbol{U}(\boldsymbol{x},t) - \boldsymbol{V}\big) U_i(\boldsymbol{x},t)}{\Delta x_j} \right\rangle \tag{96}$$

Now the first term on the R.H.S of (96) involves a two-point correlation between the fine grained PDF at the point $\boldsymbol{x}$ and the velocity at the point $\boldsymbol{x}+\Delta x_j$, which needs a two-point PDF to express the correlation. As an approximation (or modeling) for this two-point correlation at the limit $\Delta x_j \to 0$, we express it with the one-point PDF as follows

$$\left\langle \delta\big(\boldsymbol{U}(\boldsymbol{x},t) - \boldsymbol{V}\big) U_i(\boldsymbol{x}+\Delta x_j,t) \right\rangle = \int \delta\big(\boldsymbol{V}' - \boldsymbol{V}\big) V_i' f(\boldsymbol{V}'; \boldsymbol{x}+\Delta x_j,t)\, d\boldsymbol{V}' \tag{97}$$

Then Equation (96) becomes

$$\left\langle f' \frac{\partial U_i}{\partial x_j} \right\rangle = \lim_{\Delta x_j \to 0} \int \frac{\delta\big(\boldsymbol{V}' - \boldsymbol{V}\big) V_i' f_U(\boldsymbol{V}'; \boldsymbol{x}+\Delta x_j,t) - \delta\big(\boldsymbol{V}' - \boldsymbol{V}\big) V_i' f_U(\boldsymbol{V}'; \boldsymbol{x},t)}{\Delta x_j} d\boldsymbol{V}'$$
$$= \lim_{\Delta x_j \to 0} \left(\frac{V_i f_U(\boldsymbol{V}; \boldsymbol{x}+\Delta x_j,t) - V_i f_U(\boldsymbol{V}; \boldsymbol{x},t)}{\Delta x_j} \right) = V_i \frac{\partial f_U(\boldsymbol{V}; \boldsymbol{x},t)}{\partial x_j} \tag{98}$$

We note that Equation (98) itself is not exact correct due to the assumption made in Equation (97). On the other hand, the following integral equation is exactly correct:

$$\int \left\langle f' \frac{\partial U_i}{\partial x_j} \right\rangle d\boldsymbol{V} = \int \left\langle \frac{\partial U_i}{\partial x_j} \middle| \boldsymbol{V} \right\rangle f_U(\boldsymbol{V}; \boldsymbol{x},t)\, d\boldsymbol{V} = \frac{\partial \langle U_i \rangle}{\partial x_j} = \int V_i \frac{\partial f_U(\boldsymbol{V}; \boldsymbol{x},t)}{\partial x_j} d\boldsymbol{V} \tag{99}$$

This illustrates that the model (98) is just a sufficient condition for Equation (99) to be satisfied. Equation (98) also directly suggests

$$\left\langle \frac{\partial U_i}{\partial x_j} \middle| \boldsymbol{V} \right\rangle = V_i \frac{1}{f_U} \frac{\partial f_U}{\partial x_j} \tag{100}$$

Using the same procedure to carry out the mean on the right hand side of (94), we may obtain

$$\left\langle -\frac{\partial}{\partial V_i} \left\{ f' \left(-\frac{1}{\rho} \frac{\partial P}{\partial x_i} + \nu \frac{\partial^2 U_i}{\partial x_j \partial x_j} \right) \right\} \right\rangle = -\frac{\partial}{\partial V_i} \left(-\frac{P(V)}{\rho} \frac{\partial f_U}{\partial x_i} + \nu \frac{V_i \partial^2 f_U}{\partial x_j \partial x_j} \right) \tag{101}$$

Therefore, we obtain a closed velocity PDF equation:

$$\frac{\partial f_U}{\partial t} + V_j \frac{\partial f_U}{\partial x_j} = -\frac{\partial}{\partial V_i} \left(-\frac{P(V)}{\rho} \frac{\partial f_U}{\partial x_i} + \nu \frac{V_i \partial^2 f_U}{\partial x_j \partial x_j} \right) \tag{102}$$

Note that the conditional means appeared in the traditional PDF equations (Pope (Ref. 1)) are related to the terms on the right hand side of Equation (102). For example,

$$\left\langle f'\nu\frac{\partial^2 U_i}{\partial x_j \partial x_j}\right\rangle = f_U\cdot\left\langle \nu\frac{\partial^2 U_i}{\partial x_j \partial x_j}\middle| \boldsymbol{V}\right\rangle = \nu\frac{V_i\,\partial^2 f_U}{\partial x_j \partial x_j}$$

This indicates that the conditional mean is

$$\left\langle \nu\frac{\partial^2 \boldsymbol{U}_i}{\partial x_j \partial x_j}\middle| \boldsymbol{V}\right\rangle = \nu\frac{V_i}{f_U}\frac{\partial^2 f_U}{\partial x_j \partial x_j} \tag{103}$$

Similarly,

$$\left\langle \frac{1}{\rho}\frac{\partial P}{\partial x_i}\middle| \boldsymbol{V}\right\rangle = \frac{1}{\rho}\frac{\partial\left[P(\boldsymbol{V})\,f_U\right]}{f_U\ \partial x_i} \tag{104}$$

It is clear that these conditional means are actually the functional forms for $\nabla^2 U_i$ and ∇P in the sample space $\boldsymbol{V}$. Let us denote them as $L(V_i)$ and $P_i^g(V)$, then the velocity PDF equation can be simply written as

$$\begin{gathered}\frac{\partial f_U}{\partial t} + V_j\frac{\partial f_U}{\partial x_j} = -\frac{\partial}{\partial V_i}\left(-\frac{P_i^g(V)}{\rho}f_U + \nu L(V_i)\,f_U\right)\\ P_i^g(V) = \frac{1}{f_U}\frac{\partial\left[P(V)\,f_U\right]}{\partial x_i}, \qquad L(V_i) = V_i\frac{\nabla^2 f_U}{f_U}\end{gathered} \tag{105}$$

Now, let us apply the fine grained PDF to the Poison equation of $P(\boldsymbol{x},t)$, which will lead to a functional form of $P(V)$:

$$\frac{1}{\rho}\left\langle f'\nabla^2 P\right\rangle = -\left\langle f'\frac{\partial^2 U_i U_j}{\partial x_i \partial x_j}\right\rangle \tag{106}$$

The operation of the above mean, under a similar assumption made in Equation (97), gives the following equation for $P(V)$

$$\frac{\nabla^2\left[P(V)\,f_U\right]}{\rho} = -V_i V_j\frac{\partial^2 f_U}{\partial x_i \partial x_j} \tag{107}$$

A.3 Transport Equation for Joint Species-Velocity PDF $f_{u,\Phi}(\boldsymbol{V},\psi;\ \boldsymbol{x},t)$

Similar to Equation (94), the transport equation for the fine grained species PDF $f'(\psi;\ \boldsymbol{x},t) \equiv \delta\left(\Phi(\boldsymbol{x},t) - \psi\right)$ is

$$\frac{\partial f'}{\partial t} + U_j\frac{\partial f'}{\partial x_j} = -\frac{\partial}{\partial \psi_i}\left(f'\Gamma\frac{\partial^2 \Phi_i}{\partial x_j \partial x_j} - f'S_i(\Phi_1\Phi_2\cdots)\right) \tag{108}$$

Analogy to the derivation of velocity PDF equation, we may construct the following species PDF equation:

$$
\begin{aligned}
&\frac{\partial f_\Phi}{\partial t} + \frac{\partial}{\partial x_j}\left(f_\Phi \left\langle U_j \middle| \psi \right\rangle \right) = -\frac{\partial}{\partial \psi_i}\left(\Gamma\, L(\psi_i)\, f_\Phi - S_i(\psi_1 \psi_2 \cdots)\, f_\Phi \right) \\
&L(\psi_i) = \psi_i \frac{\nabla^2 f_\Phi}{f_\Phi}
\end{aligned}
\tag{109}
$$

It should also be recognized that the conditional mean $\left\langle \nabla^2 \Phi_i \middle| \psi \right\rangle$ appearing in the traditional PDF equation is represented by $L(\psi_i)$ here in Equation (109). Finally, Equations (105) and (109) will lead to a joint species-velocity PDF equation as the following:

$$
\frac{\partial f_{U,\Phi}}{\partial t} + V_j \frac{\partial f_{U,\Phi}}{\partial x_j} = -\frac{\partial}{\partial V_i}\left(-\frac{P_i^g(V)}{\rho} f_{U,\Phi} + \nu L(V_i)\, f_{U,\Phi} \right) - \frac{\partial}{\partial \psi_i}\left(\Gamma L(\psi_i)\, f_{U,\Phi} - S_i(\psi_1 \psi_2 \cdots)\, f_{U,\Phi} \right) \tag{110}
$$

Where,

$$
P_i^g(V) = \frac{1}{f_{U,\Phi}} \frac{\partial \left[P(V)\, f_{U,\Phi} \right]}{\partial x_i}, \quad L(V_i) = V_i \frac{\nabla^2 f_{U,\Phi}}{f_{U,\Phi}}, \quad L(\psi_i) = \psi_i \frac{\nabla^2 f_{U,\Phi}}{f_{U,\Phi}}
$$

Appendix B.—Miscellaneous Formulations

In the derivation of PDF equations, the following relationships have been intensively used. The proof of Equation (111) has been described by Pope (Ref. 1). The same procedure can be followed to prove Equation (112).

$$\int \frac{\partial}{\partial V_j}\left(f_U(\boldsymbol{V};\boldsymbol{x},t) A_i(\boldsymbol{V})\right) d\boldsymbol{V} = 0 \tag{111}$$

Where $A_i(\boldsymbol{V})$ is a vector function of sample space variable $\boldsymbol{V}$, and it has a finite mean.

$$\int \frac{\partial}{\partial \psi_j}\left[f_\Phi(\psi;\boldsymbol{x},t) A_i(\psi)\right] d\psi = 0 \tag{112}$$

Where $A_i(\psi)$ is a vector function of sample space variable ψ, and it has a finite mean.

Therefore, the following integrations are all zero:

$$\int \frac{\partial}{\partial V_j}\left(\left\langle -\frac{1}{\rho}\frac{\partial P}{\partial x_j}\middle| \boldsymbol{V} \right\rangle f_U(\boldsymbol{V};\boldsymbol{x},t) V_i \right) d\boldsymbol{V} = 0$$

$$\int -\frac{1}{\rho}\frac{\partial}{\partial V_j}\left(V_i \left[P(\boldsymbol{V}) f_U(\boldsymbol{V};\boldsymbol{x},t)\right]\right) d\boldsymbol{V} = 0$$

$$\int \frac{\partial}{\partial V_j}\left(V_i f_U(\boldsymbol{V};\boldsymbol{x},t) \left\langle \nu \nabla^2 U_i \middle| \boldsymbol{V} \right\rangle \right) d\boldsymbol{V} = 0$$

$$-\frac{1}{\rho}\int \frac{\partial}{\partial V_j}\left(V_i\, P_j^g(\boldsymbol{V})\, f_U(\boldsymbol{V};\boldsymbol{x},t)\right) d\boldsymbol{V} = 0.$$

$$\nu \int \frac{\partial}{\partial V_j}\left(V_i\, L(V_j)\, f_U(\boldsymbol{V};\boldsymbol{x},t)\right) d\boldsymbol{V} = 0.$$

$$\int \frac{\partial}{\partial \psi_j}\left[\psi_i f_\Phi(\psi;\boldsymbol{x},t) \left\langle \nabla^2 \Phi_j \middle| \psi \right\rangle \right] d\psi = 0$$

$$\int\int \frac{\partial}{\partial \psi_j}\left(\psi_i S_j(\psi_1\psi\cdots\psi_n)\, f_{U,\Phi}(\boldsymbol{V},\psi;x_i,t)\right) d\boldsymbol{V} d\psi = 0$$

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13. SUPPLEMENTARY NOTES

14. ABSTRACT
Recently we have revisited the traditional probability density function (PDF) equations for the velocity and species in turbulent incompressible flows. They are all unclosed due to the appearance of various conditional means which are modeled empirically. However, we have observed that it is possible to establish a closed velocity PDF equation and a closed joint velocity and species PDF equation through conditions derived from the integral form of the Navier-Stokes equations. Although, in theory, the resulted PDF equations are neither general nor unique, they nevertheless lead to the exact transport equations for the first moment as well as all higher order moments. We refer these PDF equations as the conservational PDF equations. This observation is worth further exploration for its validity and CFD application.

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