Velocity-scalar filtered density function for large eddy simulation of turbulent flows

M. R. H. Sheikhi, T. G. Drozda, and P. Givi
Department of Mechanical Engineering, University of Pittsburgh, Pittsburgh, Pennsylvania 15261

S. B. Pope
Sibley School of Mechanical and Aerospace Engineering, Cornell University, Ithaca, New York 14853-1301

(Received 7 October 2002; accepted 22 April 2003; published 2 July 2003)

A methodology termed the “velocity-scalar filtered density function” (VSFDF) is developed and implemented for large eddy simulation (LES) of turbulent flows. In this methodology, the effects of the unresolved subgrid scales (SGS) are taken into account by considering the joint probability density function (PDF) of the velocity and scalar fields. An exact transport equation is derived for the VSFDF in which the effects of the SGS convection and chemical reaction are closed. The unclosed terms in this equation are modeled in a fashion similar to that typically used in Reynolds-averaged simulation procedures. A system of stochastic differential equations (SDEs) which yields statistically equivalent results to the modeled VSFDF transport equation is constructed. These SDEs are solved numerically by a Lagrangian Monte Carlo procedure in which the Itô–Gikhman character of the SDEs is preserved. The consistency of the proposed SDEs and the convergence of the Monte Carlo solution are assessed by comparison with results obtained by a finite difference LES procedure in which the corresponding transport equations for the first two SGS moments are solved. The VSFDF results are compared with those obtained by the Smagorinsky model, and all the results are assessed via comparison with data obtained by direct numerical simulation of a temporally developing mixing layer involving transport of a passive scalar. It is shown that the values of both the SGS and the resolved components of all second order moments including the scalar fluxes are predicted well by VSFDF. The sensitivity of the calculations to the model’s (empirical) constants are assessed and it is shown that the magnitudes of these constants are in the same range as those employed in PDF methods. © 2003 American Institute of Physics. [DOI: 10.1063/1.1584678]

I. INTRODUCTION

The probability density function (PDF) approach has proven useful for large eddy simulation (LES) of turbulent reacting flows. The formal means of conducting such LES is by considering the “filtered density function” (FDF) which is essentially the filtered fine-grained PDF of the transport quantities. In all previous contributions, the “marginal” FDF of the scalars, or the marginal FDF of the velocity vector are considered; see Givi for a recent review.

The objective of the present work is to extend the FDF methodology to account for the “joint” subgrid scale (SGS) velocity and scalar fields. This is accomplished by considering the joint “velocity-scalar filtered density function” (VSFDF). With the definition of the VSFDF, the mathematical framework for its implementation in LES is established. A transport equation is developed for the VSFDF in which the effects of SGS convection and SGS chemical reaction (in a reacting flow) are closed. The unclosed terms in this equation are modeled in a fashion similar to those in the Reynolds-averaged simulation (RAS) procedures. A Lagrangian Monte Carlo procedure is developed and implemented for numerical simulation of the modeled VSFDF transport equation. The consistency of this procedure is assessed by comparing the first two moments of the VSFDF with those obtained by the Eulerian finite difference solutions of the same moments’ transport equations. The results of the VSFDF simulations are compared with those predicted by the Smagorinsky closure. All the results are assessed via comparison with direct numerical simulation (DNS) data of a three-dimensional (3D) temporally developing mixing layer involving transport of a passive scalar variable. The sensitivity of VSFDF predictions to the values of the model’s (empirical) constants is assessed.

II. FORMULATION

For the general formulation, we consider an incompressible (unit density), isothermal, turbulent reacting flow involving \( N_s \) species. The primary transport variables describing such a flow are the three components of the velocity vector \( u_i(x,t) \) \( (i = 1, 2, 3) \), the pressure \( p(x,t) \), and the species’ mass fractions \( \phi_{\alpha}(x,t) \) \( (\alpha = 1, 2, \ldots, N_s) \). The equations which govern the transport of these variables in space \( (x_i) \) and time \( (t) \) are

\[ \begin{align*}
\end{align*} \]
\[
\frac{\partial u_k}{\partial x_k} = 0, \quad (1a)
\]

\[
\begin{align*}
\frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_k} &= - \frac{\partial p}{\partial x_i} + \frac{\partial \sigma_{ik}}{\partial x_k}, \\
\frac{\partial \phi_\alpha}{\partial t} + \frac{\partial u_i \phi_\alpha}{\partial x_k} &= - \frac{\partial J^\alpha}{\partial x_k} + S_\alpha, 
\end{align*}
\]

\[(1b)\]

where \( S_\alpha = \tilde{S}_\alpha(\phi(x,t)) \) denotes the chemical reaction term for species \( \alpha \), and \( \phi = [\phi_1, \phi_2, \ldots, \phi_N] \) denotes the scalar variable array. For an incompressible, Newtonian fluid, with Fick’s law of diffusion, the viscous stress tensor \( \sigma_{ik} \) and the scalar flux \( J^\alpha_k \) are represented by

\[
\sigma_{ik} = \nu \left( \frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i} \right), \quad (2a)
\]

\[
J^\alpha_k = -\Gamma \frac{\partial \phi_\alpha}{\partial x_k}, \quad (2b)
\]

where \( \nu \) is the fluid kinematic viscosity and \( \Gamma = \nu / \text{Sc} \) is the diffusion coefficient of all species with \( \text{Sc} \) denoting the molecular Schmidt number. We assume a constant value for \( \nu = \Gamma \); i.e., \( \text{Sc} = 1 \). In reactive flows, molecular processes are much more complicated than portrayed by Eq. (2). Since the molecular diffusion is typically less important than that of SGS, this simple model is adopted with justifications and caveats given in Refs. 19–21.

Large eddy simulation involves the spatial filtering operation.

\[
(f(x,t)) = \int_{-\infty}^{+\infty} f(x',t)G(x',x)dx',
\]

\[(3)\]

where \( G(x',x) \) denotes a filter function, and \( \langle f(x,t) \rangle \) is the filtered value of the transport variable \( f(x,t) \). We consider a filter function that is spatially and temporally invariant and localized, thus: \( G(x',x) = G(x' - x) \) with the properties \( G(x) \equiv 0, \int_{-\infty}^{+\infty} G(x)dx = 1 \). Applying the filtering operation to Eqs. (1) yields

\[
\begin{align*}
\frac{\partial (u_k)}{\partial x_k} &= 0, \\
\frac{\partial (u_i)}{\partial t} + \frac{\partial (u_i u_j)}{\partial x_k} &= - \frac{\partial (p)}{\partial x_i} + \nu \frac{\partial ^2 (u_i)}{\partial x_k \partial x_k} - \frac{\partial (u_i u_j)}{\partial x_k}, \\
\frac{\partial (\phi_\alpha)}{\partial t} + \frac{\partial (u_i \phi_\alpha)}{\partial x_k} &= \nu \frac{\partial ^2 (\phi_\alpha)}{\partial x_k \partial x_k} - \frac{\partial (u_i \phi_\alpha)}{\partial x_k} + \langle S_\alpha \rangle,
\end{align*}
\]

\[(4a, b, c)\]

where the second-order SGS correlations

\[
\tau(a,b) = \langle ab \rangle - \langle a \rangle \langle b \rangle
\]

\[(5)\]

are governed by

\[
\frac{\partial \tau(u_i, u_j)}{\partial t} + \frac{\partial \tau(u_i, u_j)}{\partial x_k} = \nu \frac{\partial ^2 \tau(u_i, u_j)}{\partial x_k \partial x_k} - \tau(u_k, u_i) \frac{\partial (u_j)}{\partial x_k} - \tau(u_k, u_j) \frac{\partial (u_i)}{\partial x_k} - 2 \nu \tau \left( \frac{\partial u_i}{\partial x_k}, \frac{\partial u_j}{\partial x_k} \right) + \tau \left( \frac{\partial u_i}{\partial x_k}, \frac{\partial u_j}{\partial x_k} \right) + \tau \left( \frac{\partial u_i}{\partial x_k}, \frac{\partial u_j}{\partial x_k} \right)
\]

\[(6a)\]

and

\[
\frac{\partial \tau(\phi_\alpha, \phi_\beta)}{\partial t} + \frac{\partial \tau(\phi_\alpha, \phi_\beta)}{\partial x_k} = \nu \frac{\partial ^2 \tau(\phi_\alpha, \phi_\beta)}{\partial x_k \partial x_k} - \tau(u_k, \phi_\alpha) \frac{\partial (\phi_\beta)}{\partial x_k} - \tau(u_k, \phi_\beta) \frac{\partial (\phi_\alpha)}{\partial x_k} - 2 \nu \tau \left( \frac{\partial \phi_\alpha}{\partial x_k}, \frac{\partial \phi_\beta}{\partial x_k} \right) + \tau \left( \frac{\partial \phi_\alpha}{\partial x_k}, \frac{\partial \phi_\beta}{\partial x_k} \right) + \tau \left( \frac{\partial \phi_\alpha}{\partial x_k}, \frac{\partial \phi_\beta}{\partial x_k} \right)
\]

\[(6b)\]

In this equation, the third-order correlations

\[
\tau(a,b,c) = \langle abc \rangle - \langle a \rangle \langle bc \rangle - \langle b \rangle \langle ac \rangle - \langle c \rangle \langle ab \rangle - \langle a \rangle \langle b \rangle \langle c \rangle
\]

\[(7)\]

are uncorrelated along with the other terms within square brackets.

**III. VELOCITY-SCALAR FILTERED DENSITY FUNCTION (VSFDF)**

**A. Definitions**

The “velocity-scalar filtered density function” (VSFDF), denoted by \( P \), is formally defined as

\[
P(v, \psi; u, x,t) = \int_{-\infty}^{+\infty} \tilde{P}(v, \psi; u(x',t), \phi(x',t))G(x' - x)dx',
\]

\[(8)\]

\[
\tilde{P}(v, \psi; u, x,t) = \prod_{i=1}^{3} \delta(u_i - u_i(x,t)) \prod_{\alpha} b(\psi_\alpha - \phi_\alpha(x,t)),
\]

\[(9)\]
where \( \delta \) denotes the delta function, and \( \mathbf{v}, \mathbf{\psi} \) are the velocity vector and the scalar array in the sample space. The term \( \mathcal{Q} \) is the “fine-grained” density,\(^{20,26} \) hence Eq. (8) defines VSDF as the spatially filtered value of the fine-grained density. With the condition of a positive filter kernel,\(^{27} \) \( P \) has all of the properties of the PDF.\(^{20} \) For further developments it is useful to define the “conditional filtered value” of the variable \( \mathcal{Q}(\mathbf{x}, t) \) as

\[
\langle \mathcal{Q}(\mathbf{x}, t)|\mathbf{u}(\mathbf{x}, t) = \mathbf{\psi} \rangle = \langle \mathcal{Q}|\mathbf{v}, \mathbf{\psi} \rangle = \int_{-\infty}^{\infty} \mathcal{Q}(\mathbf{v}, \mathbf{\psi}; \mathbf{x}', t) G(\mathbf{x}' - \mathbf{x})d\mathbf{x}' \]

\[
P(\mathbf{v}, \mathbf{\psi}, \mathbf{x})
\]

Equation (10) implies the following:

\( i \quad \) for \( \mathcal{Q}(\mathbf{x}, t) = \mathbf{c} \), \( \langle \mathcal{Q}(\mathbf{x}, t)|\mathbf{v}, \mathbf{\psi} \rangle = \mathbf{c} \),

\( ii \quad \) for \( \mathcal{Q}(\mathbf{x}, t) = \hat{\mathcal{Q}}(\mathbf{u}(\mathbf{x}, t), \mathbf{\phi}(\mathbf{x}, t)) \),

\[
\langle \mathcal{Q}(\mathbf{x}, t)|\mathbf{v}, \mathbf{\psi} \rangle = \hat{\mathcal{Q}}(\mathbf{v}, \mathbf{\psi}).
\]

\( iii \quad \) Integral properties,

\[
\langle \mathcal{Q}(\mathbf{x}, t) \rangle = \int_{-\infty}^{\infty} \langle \mathcal{Q}(\mathbf{x}, t)|\mathbf{v}, \mathbf{\psi} \rangle P(\mathbf{v}, \mathbf{\psi}, \mathbf{x})d\mathbf{v} d\mathbf{\psi}.
\]

This is an exact transport equation for the VSDF. It is observed that the effects of convection [second term on left-hand side (LHS)] and chemical reaction [the second term on right-hand side (RHS)] appear in closed forms. The unclosed terms denote convective effects in the velocity-scalar sample space. Alternatively, the VSDF equation can be expressed as

\[
\frac{\partial \mathcal{Q}}{\partial t} + \frac{\partial \mathbf{u}_k \mathcal{Q}}{\partial x_k} = \frac{\partial \mathcal{Q}}{\partial t} - \frac{\partial \mathbf{u}_k \mathcal{Q}}{\partial x_k} + \mathcal{Q}(\mathbf{x}, t) - \frac{S_a(\mathbf{\psi})}{\partial \mathbf{\psi}}
\]

\( (13) \)

Integration of this according to Eq. (8) while employing Eq. (10) results in

\[
\frac{\partial \mathcal{P}}{\partial t} + \frac{\partial \mathbf{u}_k \mathcal{P}}{\partial x_k} = \frac{\partial \mathbf{p}}{\partial x_k} - \frac{\partial \mathbf{u}_k \mathcal{P}}{\partial x_k} + \mathcal{Q}(\mathbf{x}, t) - \frac{S_a(\mathbf{\psi})}{\partial \mathbf{\psi}}
\]

\( (14) \)

B. VSDF transport equations

To develop the VSDF transport equation, we consider the time derivative of the fine-grained density function [Eq. (9)],

\[
\frac{\partial \mathcal{Q}}{\partial t} = -\left( \frac{\partial \mathbf{u}_k \mathcal{Q}}{\partial x_k} + \frac{\partial \mathbf{\psi}}{\partial x_k} \right)
\]

\( (11) \)

Substituting Eqs. (1b) and (1c), and Eqs. (2a) and (2b) into Eq. (13) we obtain

\[
\frac{\partial \mathcal{P}}{\partial t} + \frac{\partial \mathbf{u}_k \mathcal{P}}{\partial x_k} = \frac{\partial \mathbf{p}}{\partial x_k} - \frac{\partial \mathbf{u}_k \mathcal{P}}{\partial x_k} + \mathcal{Q}(\mathbf{x}, t) - \frac{S_a(\mathbf{\psi})}{\partial \mathbf{\psi}}
\]

\( (14) \)

Integration of this according to Eq. (8), while employing Eq. (10) results in

\[
\frac{\partial \mathcal{P}}{\partial t} + \frac{\partial \mathbf{u}_k \mathcal{P}}{\partial x_k} = \frac{\partial \mathbf{p}}{\partial x_k} - \frac{\partial \mathbf{u}_k \mathcal{P}}{\partial x_k} + \mathcal{Q}(\mathbf{x}, t) - \frac{S_a(\mathbf{\psi})}{\partial \mathbf{\psi}}
\]

\( (15) \)

This is also an exact equation, but the unclosed terms are exhibited by the conditional filtered values of the dissipation fields as shown by the last three terms on the RHS.

C. Modeled VSDF transport equation

For closure of the VSDF transport equation, we consider the general diffusion process,\(^{28} \) given by the system of stochastic differential equations (SDEs):

\[
dX^+_i(t) = D^+_i(X^+, U^+, \mathbf{\phi}^+; t)dt
\]

\[
+ B^+_i(X^+, U^+, \mathbf{\phi}^+; t)dW^+_i(t)
\]

\[
+ F^+_iU^+ (X^+, U^+, \mathbf{\phi}^+; t)dW^+_j(t)
\]

\[
+ F^+_iU^+ (X^+, U^+, \mathbf{\phi}^+; t)dW^+_j(t),
\]

\( (17a) \)

\[
dU^+_i(t) = D^+_i(X^+, U^+, \mathbf{\phi}^+; t)dt
\]

\[
+ B^+_i(X^+, U^+, \mathbf{\phi}^+; t)dW^+_i(t)
\]

\[
+ F^+_iU^+ (X^+, U^+, \mathbf{\phi}^+; t)dW^+_j(t)
\]

\[
+ F^+_iU^+ (X^+, U^+, \mathbf{\phi}^+; t)dW^+_j(t),
\]

\( (17b) \)
The transport equations for the second-order SGS moments are

\[ d\phi_a^+ = \int \left[ \frac{\partial^2 (\phi_a)}{\partial x_k \partial x_k} - C_\phi (\phi_a^+ - \langle \phi_a \rangle) + S_a \right] dt + \sqrt{\nu_2} \frac{\partial (\phi_a)}{\partial x_k} dW_k^\xi, \]  

where the variables \( \nu_1, \nu_2, \ldots \) are all diffusion coefficients (to be specified), and

\[ G_{ij} = -\omega \left[ \frac{1}{2} + \frac{3}{4} C_0 \right] \delta_{ij}, \quad \omega = \frac{e}{k}, \]  

Here \( \omega \) is the SGS mixing frequency, \( e \) is the SGS dissipation rate, \( k \) is the SGS kinetic energy, and \( \Delta_L \) is the LES filter size. The parameters \( C_0, C_\phi, C_\epsilon \) are model constants and need to be specified. The limit \( \nu_1 = \nu_3 = \nu_5 = \nu_7 = 0 \) is the standard high Reynolds number GLM–LMSE closure.

The Fokker–Planck equation for \( f(v, \psi, \mathbf{x}; t) \), the joint PDF of \( \mathbf{X}^+, \mathbf{U}^+, \mathbf{\phi}^+ \), evolving by the diffusion process as given by Eq. (18) is

\[
\frac{\partial f}{\partial t} + \frac{\partial}{\partial x_i} (v_i f) = \left[ \frac{\partial (p)}{\partial x_i} - (v_2 - \sqrt{v_1 v_3}) \frac{\partial^2 (u_i)}{\partial x_k \partial x_k} \right] \frac{\partial f}{\partial v_i} + \frac{\partial}{\partial \psi_a} \left[ C_\phi (\psi_a - \langle \psi_a \rangle) f \right] + \frac{\partial}{\partial \psi_a} \left[ S_a (\psi) f \right] + \nu_1 \frac{\partial^2 f}{\partial x_i \partial x_k} + \sqrt{v_1 v_3} \frac{\partial (u_i)}{\partial x_k} \frac{\partial f}{\partial v_j} \frac{\partial^2 f}{\partial x_i \partial v_j} + \frac{1}{2} C_0 \epsilon \frac{\partial^2 f}{\partial v_k \partial \psi_a} + \nu_3 \frac{\partial (u_i)}{\partial x_k} \frac{\partial (\phi_a)}{\partial v_k} \frac{\partial^2 f}{\partial x_i \partial v_k} + \frac{\partial (u_i)}{\partial x_k} \frac{\partial (\phi_a)}{\partial \psi_a} \frac{\partial f}{\partial v_k} \frac{\partial^2 f}{\partial x_i \partial \psi_a} + \frac{\partial (u_i)}{\partial x_k} \frac{\partial (\phi_a)}{\partial \psi_a} \frac{\partial f}{\partial \psi_a} \frac{\partial^2 f}{\partial x_i \partial \psi_a}.
\]

The transport equations for the filtered variables are obtained by integration of Eq. (20) according to Eq. (12):

\[
\frac{\partial (u_k)}{\partial x_k} = 0,
\]

\[
\frac{\partial (u_i)}{\partial t} + \frac{\partial (u_j)}{\partial x_k} (u_i) = -\frac{\partial (p)}{\partial x_i} \frac{\partial^2 (u_i)}{\partial x_k \partial x_k} - \tau (u_k, u_i),
\]

\[
\frac{\partial (\phi_a)}{\partial t} + \frac{\partial (u_k)}{\partial x_k} (\phi_a) = \left[ v_1 - \sqrt{v_1 v_3} \right] \frac{\partial^2 (\phi_a)}{\partial x_k \partial x_k} + (S_a (\psi) - \tau (u_k, \phi_a)).
\]

The transport equations for the second-order SGS moments are

\[
\frac{\partial \tau (u_i, u_j)}{\partial t} + \frac{\partial (u_k)}{\partial x_k} (\tau (u_i, u_j)) = \frac{\nu_1}{2} \frac{\partial^2 \tau (u_i, u_j)}{\partial x_k \partial x_k} - \tau (u_k, u_i) \frac{\partial (u_j)}{\partial x_k} - \tau (u_k, u_j) \frac{\partial (u_i)}{\partial x_k} + (v_1 - \sqrt{v_1 v_3} + v_3) \frac{\partial (u_i)}{\partial x_k} \frac{\partial (u_j)}{\partial x_k} + \left[ G_{ik} \tau (u_k, u_j) + G_{jk} \tau (u_k, u_i) + C_0 \epsilon \delta_{ij} \right] \tau (u_k, u_j),
\]

where \( \tau (u_k, u_j) \) is the SGS kinetic energy, and \( \tau (u_k, \phi_a) \) is the SGS mixing frequency, and \( \Delta_L \) is the LES filter size. The parameters \( C_0, C_\phi, C_\epsilon \) are model constants and need to be specified. The limit \( \nu_1 = \nu_3 = \nu_5 = \nu_7 = 0 \) is the standard high Reynolds number GLM–LMSE closure.
\[
\frac{\partial (u_i, \phi_a)}{\partial t} + \frac{\partial (u_k)}{\partial x_k} \tau(u_i, \phi_a) = \frac{\nu_1}{2} \frac{\partial^2 \tau(u_i, \phi_a)}{\partial x_k \partial x_k} - \tau(u_k, u_i) \frac{\partial (u_i)}{\partial x_k} \frac{\partial (u_k)}{\partial x_k} + \frac{\tau(u_k, u_i)}{\partial x_k} \frac{\partial (u_i)}{\partial x_k} \frac{\partial (u_k)}{\partial x_k} + \left[ G_{ik} \tau(u_k, \phi_a) - C_{\phi \omega} \tau(u_i, \phi_a) \right] + \tau(u_i, S_a) - \frac{\partial \tau(u_k, u_i, \phi_a)}{\partial x_k},
\]

\[
\frac{\partial \tau(\phi_a, \phi_b)}{\partial t} + \frac{\partial (u_k)}{\partial x_k} \tau(\phi_a, \phi_b) = \frac{\nu_1}{2} \frac{\partial^2 \tau(\phi_a, \phi_b)}{\partial x_k \partial x_k} - \tau(u_k, \phi_a) \frac{\partial (\phi_b)}{\partial x_k} \frac{\partial (u_k)}{\partial x_k} + \left[ 2 C_{\phi \omega} \tau(\phi_a, \phi_b) \right] + \tau(\phi_a, S_b) + \frac{\partial \tau(u_k, \phi_a, \phi_b)}{\partial x_k}.
\]
\[
\frac{\partial \tau(\phi_a, \phi_B)}{\partial t} + \frac{\partial(u_k) \tau(\phi_a, \phi_B)}{\partial x_k} = \nu \frac{\partial^2 \tau(\phi_a, \phi_B)}{\partial x_k \partial x_k} - \tau(u_k, \phi_a) \frac{\partial(\phi_B)}{\partial x_k} - \tau(u_k, \phi_B) \frac{\partial(\phi_a)}{\partial x_k} + 2 \nu \frac{\partial(\phi_a)}{\partial x_k} \frac{\partial(\phi_B)}{\partial x_k} - 2 \nu \frac{\partial^2 \tau(\phi_a, \phi_B)}{\partial x_k \partial x_k} - \tau(\phi_a, S_B) + \tau(\phi_B, S_a) - \frac{\partial(\phi_a) \frac{\partial(\phi_B)}{\partial x_k}}{\partial x_k}
\]

which may be compared to Eqs. (4) and (6). Therefore, the stochastic diffusion process described by the SDEs (23) implies the following closure for the VSFDF:

\[
\frac{\partial}{\partial x_k} \left[ \left( \frac{\partial p}{\partial x_k} v, \psi \right) - \frac{\partial(p)}{\partial x_k} P \right] - \nu \frac{\partial^2}{\partial x_k \partial x_k} \left[ \left( \frac{\partial u_i}{\partial x_k} \frac{\partial u_j}{\partial x_k} v, \psi \right) P \right] - 2 \nu \frac{\partial^2}{\partial x_k \partial x_k} \left[ \left( \frac{\partial u_i}{\partial x_k} \frac{\partial u_j}{\partial x_k} v, \psi \right) P \right] - \frac{\partial(\phi_a) \frac{\partial(\phi_B)}{\partial x_k}}{\partial x_k} \left( \left( \frac{\partial u_i}{\partial x_k} \frac{\partial u_j}{\partial x_k} v, \psi \right) P \right) - \frac{\partial G_{ij}(v_j - \langle u_j \rangle)}{\partial x_k} \left( \frac{\partial \psi_a}{\partial x_k} \left( \frac{\partial \phi_a}{\partial x_k} \right) \right) P
\]

which yields the closures at the second-order levels:

\[
\begin{align*}
- \nu & \left( \frac{\partial u_i}{\partial x_k} \frac{\partial u_j}{\partial x_k} v, \psi \right) + \tau(u_i, \phi_a) + \tau(u_j, \phi_B) \\
& = G_{ik} \tau(u_k, u_i) + G_{jk} \tau(u_k, u_j) + C_0 \delta_{ij} \\
& = -\omega(1 + \frac{1}{2} C_0) \left[ \tau(u_i, u_j) - \frac{2}{3} \delta_{ij} \right] - \frac{2}{3} \epsilon \delta_{ij},
\end{align*}
\]

\[
\begin{align*}
- \nu & \left( \frac{\partial u_i}{\partial x_k} \frac{\partial \phi_a}{\partial x_k} v, \psi \right) + \tau(u_i, \phi_a) \\
& = G_{ik} \tau(u_k, \phi_a) - C_\phi \omega \tau(u_i, \phi_a) \\
& = -\omega \left( \frac{1}{2} + \frac{3}{4} C_0 + C_\phi \right) \tau(u_i, \phi_a),
\end{align*}
\]

\[
\begin{align*}
- \nu & \left( \frac{\partial \phi_a}{\partial x_k} \frac{\partial \phi_B}{\partial x_k} v, \psi \right) \\
& = -2 C_\phi \omega \tau(\phi_a, \phi_B) + 2 \nu \frac{\partial(\phi_a)}{\partial x_k} \frac{\partial(\phi_B)}{\partial x_k}.
\end{align*}
\]

IV. NUMERICAL SOLUTION PROCEDE

Numerical solution of the modeled VSFDF transport equation is obtained by a hybrid finite difference-Monte Carlo procedure. The basis is similar to those in RAS34–36 and in previous FDF simulations,7,9,16 with some differences which are described here. For simulations, the FDF is represented by an ensemble of N_p statistically identical Monte Carlo (MC) particles. Each particle carries information pertaining to its position, (X^{(n)}(t), velocity, (u^{(n)}(t), and scalar value, (\phi^{(n)}(t), n = 1,..,N_p. This information is updated via temporal integration of the SDEs. The simplest way of performing this integration is via Euler–Maruyamma approximation.37 For example, for Eq. (17a),

\[
X^{n+1}(t_k+1) = X^n(t_k) + (D^X(t_k))^{n} \Delta t + (B^{X^2}_{ij}(t_k))^n (\Delta t)^{1/2} (\xi^X_{ij}(t_k))^{n} + (F^{XX^2}_{ij}(t_k))^n (\Delta t)^{1/2} (\xi^{XX^2}_{ij}(t_k))^{n},
\]

where (X^{n}(t_k), (u^{(n)}(t_k), (\phi^{(n)}(t_k),... and \xi(t_k)’s are independent standardized Gaussian random variables. This scheme preserves the Itô character of the SDEs.38

The computational domain is discretized on equally spaced finite difference grid points. These points are used for two purposes: (1) to identify the regions where the statistical

FIG. 1. Concept of ensemble averaging in 2D. Shown are three different ensemble domains: 1(\Delta_x = \Delta/2, N_x = 10), 2(\Delta_x = \Delta, N_x = 40), 3(\Delta_x = 2\Delta, N_x = 160). Solid squares denote the finite-difference grid points, and the circles denote the MC particles.
information from the MC simulations are obtained; (2) to perform LES primarily by the finite difference methodology which is coupled to the MC solver. The LES procedure via the finite difference discretization is referred to as LES–FD and will be further discussed below.

Statistical information is obtained by considering an ensemble of $N_E$ computational particles residing within an ensemble domain of characteristic length $\Delta_E$ centered around each of the finite-difference grid points. This is illustrated schematically in Fig. 1. For reliable statistics with minimal numerical dispersion, it is desired to minimize the size of ensemble domain and maximize the number of the MC particles. In this way, the ensemble statistics would tend to the desired filtered values,

$$\langle a \rangle_{E} = \frac{1}{N_E} \sum_{n=1}^{N_E} a^{(n)} \frac{\Delta E}{\Delta E} \approx \langle a \rangle,$$

(30)

where $a^{(n)}$ denotes the information carried by nth MC particle pertaining to transport variable $a$.

The LES–FD solver is based on the compact parameter finite difference scheme. This is a variant of the MacCormack scheme in which fourth-order compact differencing schemes are used to approximate the spatial derivatives, and second-order symmetric predictor–corrector sequence is employed for time discretization. All of the finite difference operations are conducted on fixed grid points. The transfer of information from the grid points to the MC particles is accomplished via a second-order interpolation. The transfer of information from the particles to the grid points is accomplished via ensemble averaging as described above.

The LES–FD procedure determines the pressure field which is used in the MC solver. The LES–FD also determines the filtered velocity and scalar fields. That is, there is a “redundancy” in the determination of the first filtered moments as both the LES–FD and the MC procedures provide the solution of this field. This redundancy is actually very useful in monitoring the accuracy of the simulated results as shown in previous work. To establish consistency and convergence of the MC solver, the modeled transport equations for the generalized second-order SGS moments [Eq. (26)] are also solved via LES–FD. In doing so, the unclosed third-order correlations are taken from the MC solver. The comparison of the first and second-order moments as obtained by LES–FD with those obtained by the MC solver is useful to establish the accuracy of the MC solver. These simulations are referred to as VSFDF–C. Attributes of all the simulation procedures are summarized in Table I. In this table and hereinafter, VSFDF simulations refer to the hybrid MC/LES–FD procedure in which the LES–FD is used for only the first-order filtered variables. In VSFDF–C, the LES–FD procedure is used for both first- and second-order filtered values. Further discussions about the simulation methods are available in Refs. 7, 16, 34–36.

V. RESULTS

A. Flows simulated

Simulations are conducted of a two-dimensional (2D) and a 3D incompressible, temporally developing mixing layers involving transport of a passive scalar variable. Since the performance of the model in capturing the velocity-scalar correlations is of primary interest, only nonreacting flow simulations are conducted. Inclusion of chemical reaction via the joint FDF formulation is straightforward and is similar to that in the marginal scalar FDF method. The 2D simulations are performed to establish and demonstrate the consistency of the MC solver. The 3D simulations are used to assess the overall predictive capabilities of the VSFDF methodology. These predictions are compared with data obtained by direct numerical simulation (DNS) of the same layer.

The temporal mixing layer consists of two parallel streams travelling in opposite directions with the same speed. In the representation below, $x$, $y$ (and $z$) denote the streamwise, the cross-stream (and the spanwise) directions (in 3D), respectively. The velocity components along these directions are denoted by $u$, $v$ (and $w$) in the $x$, $y$ (and $z$) directions, respectively. Both the filtered streamwise velocity and the scalar fields are initialized with a hyperbolic tangent profiles with $\langle u \rangle = 1$, $\langle \phi \rangle = 1$ on the top stream and $\langle u \rangle = -1$, $\langle \phi \rangle = 0$ on the bottom stream. The length $L$ is specified such that $L = 2N_P \Delta x_u$, where $N_P$ is the desired num-

<table>
<thead>
<tr>
<th>Table I. Attributes of the computational methods.</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>LES-FD</strong></td>
</tr>
<tr>
<td>-----------</td>
</tr>
<tr>
<td>$\langle p \rangle$</td>
</tr>
<tr>
<td>$\langle \phi \rangle$</td>
</tr>
<tr>
<td>$\tau(u_1, u_i)$</td>
</tr>
<tr>
<td>$\tau(u_1, \phi_n)$</td>
</tr>
<tr>
<td>$\tau(\phi_n, \phi_n)$</td>
</tr>
</tbody>
</table>
ber of successive vortex pairings and \( \lambda_u \) is the wavelength of the most unstable mode corresponding to the mean streamwise velocity profile imposed at the initial time. The flow variables are normalized with respect to the half initial vorticity thickness, \( \lambda_r = \frac{\delta_v(t=0)/2}{|\partial u/\partial y|_{\text{max}}} \), where \( \langle u \rangle_L \) is the Reynolds averaged value of the filtered streamwise velocity and \( \Delta U \) is the velocity difference across the layer. The reference velocity is \( \bar{U}_r = \Delta U/2 \).

All 2D simulations are conducted for \( 0 < x < L \), and \( -2L/3 < y < 2L/3 \). The formation of large scale structures is facilitated by introducing small harmonic, phase-shifted, disturbances containing subharmonics of the most unstable mode into the streamwise and cross-stream velocity profiles. For \( N_p = 1 \), this results in formation of two large vortices and one subsequent pairing of these vortices. The 3D simulations are conducted for a cubic box, \( 0 < x < L \), \( -L/2 < y < L/2 \) (\( 0 < z < L \)). The 3D field is parametrized in a procedure somewhat similar to that by Vreman et al.44 The formation of the large scale structures are expedited through eigenfunction based initial perturbations.45,46 This includes two-dimensional42,44,47 and three-dimensional42,48 perturbations with a random phase shift between the 3D modes. This results in the formation of two successive vortex pairings and strong three dimensionality.

**B. Numerical specifications**

Simulations are conducted on equally spaced grid points with grid spacings \( \Delta x = \Delta y = \Delta z \) (for 3D) = \( \Delta \). All 2D simulations are performed on \( 32 \times 41 \) grid points. The 3D simulations are conducted on \( 193^3 \) and \( 33^3 \) points for DNS and LES, respectively. The Reynolds number is \( \text{Re} = \bar{U}_r L_r/\nu = 50 \). To filter the DNS data, a top-hat function of the form below is used

\[
G(x') = \prod_{i=1}^{3} \tilde{G}(x'_i - x_i),
\]

\[
\tilde{G}(x'_i - x_i) = \begin{cases} 
\frac{1}{\Delta_L}, & |x'_i - x_i| \leq \frac{\Delta_L}{2}, \\
0, & |x'_i - x_i| > \frac{\Delta_L}{2}.
\end{cases}
\]

No attempt is made to investigate the sensitivity of the results to the filter function27 or the size of the filter.49

The MC particles are initially distributed throughout the computational region. All simulations are performed with a uniform “weight”20 of the particles. Due to flow periodicity in the streamwise (and spanwise in 3D) direction(s), if the particle leaves the domain at one of these boundaries new particles are introduced at the other boundary with the same velocity and compositional values. In the cross-stream directions, the free-slip boundary condition is satisfied by the mirror-reflection of the particles leaving through these boundaries. The density of the MC particles is determined by the average number of particles \( N_E \) within the ensemble domain of size \( \Delta_E \times \Delta_E \times \Delta_E \). The effects of both of these parameters are assessed to ensure the consistency and the statistical accuracy of the VSFDF simulations. All results are analyzed both “instantaneously” and “statistically.” In the former, the instantaneous contours (snap-shots) and scatter plots of the variables of interest are analyzed. In the latter,
the “Reynolds-averaged” statistics constructed from the instantaneous data are considered. These are constructed by spatial averaging over $x$ (and $z$ in 3D). All Reynolds-averaged results are denoted by an overbar.

C. Consistency and convergence assessments

The objective of this section is to demonstrate the consistency of the VSFDF formulation and the convergence of its MC simulation procedure. For this purpose, the results via MC and LES–FD are compared against each other in VSFDF–C simulations. Since the accuracy of the FD procedure is well-established (at least for the first-order filtered quantities), such a comparative assessment provides a good means of assessing the performance of the MC solution. No attempt is made to determine the appropriate values of the model constants; the values suggested in the literature are adopted\textsuperscript{50} $C_0 = 2.1$, $C_x = 1$, and $C_d = 1$. The influence of these parameters is assessed in Sec. V D.

The uniformity of the MC particles is checked by monitoring their distributions at all times, as the particle number density must be proportional to fluid density. The Reynolds averaged density fields as obtained by both LES–FD and by MC are shown in Fig. 2. Close to unity values for the density at all times is the first measure of the accuracy of simulations. Figures 3 and 4 show the instantaneous contour plots of the filtered scalar and vorticity fields at several times. These figures provide a visual demonstration of the consistency of the VSFDF. This consistency is observed for all first

---

FIG. 3. (Color) Temporal evolution of the scalar (with superimposed vorticity iso-lines) (top) and the vorticity (bottom) fields for LES–FD, with $\Delta_x = \Delta / 2$ and $N = 40$ at several times.
order moments without any statistical variability. Also, all of
these moments show very little dependence on the values of
$\Delta_E$ and $N_E$ consistent with previous FDF simulations.\textsuperscript{7,9,16} In
the presentation below we only focus on second-order mo-
ments. Specifically, the scalar-velocity correlations are
shown since all other second-order SGS moments behave
similarly.

Figures 5 and 6 show the statistical variability of the
results for simulations with $N_E=40$. It is observed that these
moments exhibit spreads with variances decreasing as the
size of the ensemble domain is reduced. Figures 7–10 show
the sensitivity to $N_E$ and $\Delta_E$. All these results clearly display
convergence suggested by Eq. (30). As the ensemble domain
size decreases, the VSFDF results converge to those of LES–
FD. Ideally, the LES–FD results should become independent
of the MC results, as the latter become more reliable, i.e.,
when ($N_E \rightarrow \infty$, $\Delta_E \rightarrow 0$). It is observed that best match is
achieved with $\Delta_E=\Delta/2$ and $N_E \geq 40$. This conclusion is con-
sistent with previous assessment studies on the scalar FDF,\textsuperscript{7,9}
and the velocity FDF.\textsuperscript{16} All the subsequent simulations are
conducted with $\Delta_E=\Delta/2$ and $N_E=40$.

\subsection*{D. Comparative assessments of the VSFDF}

The objective of this section is to analyze some of the
characteristics of the VSFDF via comparative assessments
against DNS data. In addition, comparisons are also made
with LES via the “conventional” Smagorinsky\textsuperscript{18,51} model:

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig4}
\caption{(Color) Temporal evolution of the scalar (with superimposed vorticity iso-lines) (top) and the vorticity (bottom) fields for VSFDF with $\Delta_E=\Delta/2$ and $N_E=40$ at several times.}
\end{figure}
$$\tau_L(u_i, u_j) - \frac{2}{3} k \delta_{ij} = -2 \nu_t S_{ij},$$

$$\tau_L(u_i, \phi) = -\Gamma_i \frac{\partial (\phi)_L}{\partial x_i},$$

$$S_{ij} = \frac{1}{2} \left( \frac{\partial (u_i)_L}{\partial x_j} + \frac{\partial (u_j)_L}{\partial x_i} \right),$$

$$\nu_t = C_r \Delta_L S, \quad \Gamma_i = \frac{\nu_t}{S_{ci}},$$

$$C_r = 0.04, \quad Sc_f = 1, \quad S = \sqrt{S_{ij} S_{ij}} \quad \text{and} \quad \Delta_L \text{ is the characteristic length of the filter. This model considers the anisotropic part of the SGS stress tensor } a_{ij} = \tau_L(u_i, u_j) - 2/3k \delta_{ij}. \quad \text{The isotropic components are absorbed in the pressure field.}$$

For comparison, the DNS data are transposed from the original high resolution $193^3$ points to the coarse $33^3$ points. In the comparisons, we also consider the “resolved” and the “total” components of the Reynolds-averaged moments. The

FIG. 5. Statistical variability of LES–FD and VSFDF–C simulations with $N_E = 40$ for Reynolds-averaged values of $\tau(u, \phi)$ at $t = 34.4$. Solid lines, LES–FD; dashed lines, VSFDF–C.

FIG. 6. Statistical variability of LES–FD and VSFDF–C simulations with $N_E = 40$ for Reynolds-averaged values of $\tau(u, \phi)$ at $t = 34.4$. Solid lines, LES–FD; dashed lines, VSFDF–C.

FIG. 7. Cross-stream variations of the Reynolds-averaged values of $\tau(u, \phi)$ (a) $\Delta_x = \Delta/2$, (b) $\Delta_x = \Delta$, (c) $\Delta_x = 2\Delta$. 

\[ A_E = \Delta/2 \]
former are denoted by $R(a,b)$ with $R(a,b) = \langle (a) \rangle - \langle (a) \rangle \times \langle (b) \rangle - \langle (b) \rangle$; and the latter is $r(a,b)$ with $r(a,b) = (a - \bar{a})(b - \bar{b})$. In DNS, the “total” SGS components are directly available, while in LES they are approximated by $r(a,b) \approx R(a,b) + r(a,b)$. Unless indicated otherwise, the values of the model constants are $C_0 = 2.1$, $C_x = 1$, $C_\phi = 1$; but the effects of these parameters on the predicted results are assessed.

Figure 11 shows the instantaneous iso-surface of the $\langle \phi \rangle$ field $t = 80$. By this time, the flow has gone through pairings and exhibits strong 3D effects. This is evident by the formation of large scale spanwise rollers with presence of mushroom-like structures in streamwise planes. Similar to previous results, the amount of SGS diffusion with the Smagorinsky model is significant. Thus, the predicted results are overly smooth. The Reynolds-averaged values of the filtered scalar field at $t = 80$ are shown in Fig. 12, and the temporal variation of the “scalar thickness,”

$$\delta(t) = |y(\langle \phi \rangle = 0.9)| + |y(\langle \phi \rangle = 0.1)|$$

is shown in Fig. 13. The filtered and unfiltered DNS data yield virtually indistinguishable results. The dissipative nature of the Smagorinsky model at initial times resulting in a slow growth of the layer is shown. All VSFDF predictions compare well with DNS data in predicting the spread of the layer.

Several components of the planar averaged values of the second-order SGS moments are compared with DNS data in
Figs. 14 and 15 for several values of the model constants. In general, the VSFDF results are in better agreement with DNS data than those predicted by the Smagorinsky model. In this regard, therefore, the VSFDF is expected to be more effective than the Smagorinsky type closures for LES of reacting flows since the extent of SGS mixing is heavily influenced by these SGS moments. However, it is not possible to suggest “optimum” values for the model constants, except that at small $C_v$ and $C_f$ values, the SGS energy is very large.

Several components of the resolved second-order moments are presented in Figs. 16 and 17. As expected, the performance of the Smagorinsky model is not very good as it does not predict the spread and the peak value accurately. The VSFDF yields reasonable predictions except for small $C_v$ values. However, the total values of these moments are fairly independent of the model constants and yield very good agreement with DNS data as shown in Figs. 18 and 19. It is also noted that while the SGS moments and/or the resolved moments may be overestimated and/or underestimated depending on the values of the model coefficients, the total values of the moments are fairly independent of these coefficients, at least in the range of values as considered. But
low values of $C_\phi$, $C_\epsilon$ are not recommended as they would result in too much SGS energy in comparison to the resolved energy.

The computational cost of VSFDF simulations relative to those required by DNS and by the Smagorinsky model is the same as that reported previously.\textsuperscript{16} The typical ratios of the normalized Smagorinsky–VSFDF–DNS run times are $1 - \mathcal{O}(30) - \mathcal{O}(200)$.

VI. SUMMARY AND CONCLUDING REMARKS

The filtered density function (FDF) methodology has proven effective for LES of turbulent reactive flows. In previous investigations, either the marginal FDF of the scalar, or that of the velocity were considered. The objective of present work is to develop the joint velocity-scalar FDF methodology. For this purpose, the exact transport equation governing the evolution of VSFDF is derived. It is shown that effects of the SGS convection and chemical reaction appear in a closed form. The unclosed terms are modeled in a fashion similar to those typically followed in PDF methods. The modeled VSFDF transport equation is solved numerically via a Lagrangian Monte Carlo (MC) scheme via consideration of a system of equivalent stochastic differential equations.
SDEs. These SDEs are discretized via the Euler–Maruyama approximation. The consistency of the VSFDF method and the convergence of its MC solutions are assessed in LES of a two-dimensional (2D) temporally developing mixing layer. This assessment is done by comparing the results obtained by the MC procedure with those of the finite-difference scheme (LES–FD) for the solution of the transport equations of the first two moments of VSFDF. By including the third moments from the VSFDF into the LES–FD, the consistency and convergence of the MC solution are demonstrated by good agreements of the first two SGS moments with those obtained by LES–FD.

The VSFDF predictions are compared with LES results with the Smagorinsky SGS model. All of these results are also compared with direct numerical simulation (DNS) data of a three-dimensional, temporally developing mixing layer. It is shown that the VSFDF performs well in predicting some of the phenomena pertaining to the SGS transport. Most of the overall flow features, including the mean field, the resolved and total stresses as predicted by VSFDF are in good agreement with DNS data. However, the model does require the input of three empirical constants. Also, the numerical implementation of VSFDF is more expensive than the traditional models. It may be possible to improve the predictive capabilities of the VSFDF by two ways: (1) development of a dynamic procedure to determine the model coefficients, and/or (2) implementation of higher order closures for the generalized Langevin model parameter $G_{ij}$. Future work is recommended for development and application of the joint filtered velocity-scalar mass density function (VSFMDF) to allow for LES of variable density flows with/or without the presence of chemical reaction.
ACKNOWLEDGMENTS

The authors are indebted to Dr. P. J. Colucci, Dr. T. D. Dreenben, Dr. M. Germano, Dr. L. Y. M. Gicquel, Dr. S. Heinz, Dr. M. Lesieur, Dr. H. Steiner, and Dr. C. Tong for their excellent and very valuable comments on the first draft of this manuscript. Part of this work was conducted when the first three authors were at the State University of New York at Buffalo. The work is sponsored by the U.S. Air Force Office of Scientific Research under Grant No. F49620-03-1-0022 to University of Pittsburgh and Grant No. F49620-03-1-0015 to Cornell University. Dr. Julian M. Tishkoff is the Program Manager for both these grants. Additional support for the work at University of Pittsburgh is provided by the NASA Langley Research Center under Grant No. NAG-1-03010 with Dr. J. Philip Drummond as the Technical Monitor. Computational resources are provided by the NCSA at the University of Illinois at Urbana and by the Pittsburgh Supercomputing Center (PSC).

26E. E. O’Brien, “The probability density function (PDF) approach to reacting turbulent flows,” see Libby and Williams (Ref. 19), Chap. 5, pp. 185–218.
Phys. Fluids, Vol. 15, No. 8, August 2003

References