Compressible Scalar Filtered Mass Density Function Model for High-Speed Turbulent Flows

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The scalar filtered mass density function model is further extended and employed for large-eddy simulations of high-speed turbulent mixing and reacting flows. The model is implemented through a hybrid mathematical/computational methodology. In this methodology, the filtered compressible Navier-Stokes equations in a curvilinear coordinate system are solved with a generalized, high-order, multiblock, finite difference scheme for the turbulent velocity and pressure. However, the scalar mixing and combustion are computed with the compressible scalar filtered mass density function. The pressure effect in the energy equation, as needed in high-speed flows, is included in the filtered mass density function formulation. The new compressible large-eddy simulation/filtered mass density function model is used for the simulations of flows in a rapid compression machine, in a shock tube and in a supersonic coaxial jet. The numerical results indicate that the model is able to correctly capture the scalar mixing in compressible subsonic and supersonic turbulent flows.

Nomenclature

\( C_d \) = Smagorinsky model coefficient
\( C_m \) = modified kinetic energy velocity model coefficient
\( C_w \) = mixing model coefficient
\( E \) = total energy, J/kg
\( e_c \) = internal energy, J/kg
\( \tilde{F}, \tilde{G}, \tilde{H} \) = inviscid fluxes
\( \tilde{F}, \tilde{G}, \tilde{H} \) = viscous fluxes
\( G \) = filter function
\( J \) = Jacobian of transformation
\( N_s \) = number of species
\( \bar{P}_L \) = filtered mass density function, Kg
\( Pr_f \) = turbulent Prandtl number
\( p \) = pressure, Pa
\( \bar{Q} \) = heat release rate, J/kg - s
\( R \) = mixture gas constant, J/kg · K
\( Sc \) = Schmidt number
\( S_p \) = source term vector
\( |\tilde{S}| \) = magnitude of strain rate, 1/s
\( T \) = temperature, K
\( T_{ref} \) = reference temperature, K
\( t \) = time, s
\( U \) = solution vector
\( u, v, w \) = velocity components, m/s
\( u_{ref} \) = reference velocity, m/s
\( W \) = Wiener process, \( s^{1/2} \)
\( w_{(i)} \) = weight of a Monte Carlo particle
\( X^i \) = Lagrangian position of a Monte Carlo particle, m
\( x \) = position vector, m
\( x_i \) = ith component of the position vector, m
\( \Gamma_i, \Gamma_f \) = molecular and turbulent diffusion coefficients, Kg/m · s
\( \Delta_c \) = filter size, m
\( \delta \) = Dirac delta function
\( \mu, \mu_v, \mu^* \) = molecular, effective, and artificial viscosity, respectively, Kg/m · s
\( v_i \) = subgrid-scale turbulent kinematic viscosity, m²/s
\( \xi, \eta, \xi, \tau \) = independent variables in transformed domain
\( \eta_r, \eta_i, \eta_r, \eta_i \) = metric coefficients for the coordinate transformation
\( \rho \) = density, Kg/m³
\( \sigma \) = fine-grained density
\( \Phi \) = scalar vector
\( \phi_0 \) = scalar \( \alpha \)
\( \phi_{(s)} \) = scalar value of a Monte Carlo particle
\( \Omega_m \) = composition sample space vector
\( \omega_a \) = reaction rate of species \( \alpha \), 1/s
\( \langle \cdot \rangle, \Phi \) = Favre-filtered value
\( \langle \cdot \rangle_L, \phi_{(s)} \) = conditional Favre-filtered value
\( \langle \cdot \rangle, \Phi \) = filtered value
\( \langle \cdot \rangle_f \) = secondary filter function
\( \langle \cdot \rangle \) = time-averaged value
\( \langle \cdot \rangle_v \) = conditional (volume) averaged value

Subscripts

\( i, j \) = repeated or free indices
\( \alpha \) = scalar index

I. Introduction

The performance of combustors in airbreathing propulsion systems is dependent on the complicated and often coupled effects of various factors, such as the input/output operating flow conditions, the geometry, the fuel–air mixing, and the fuel chemistry. Normally, it is difficult to predict the combustor behavior for various operating conditions. High-fidelity computational models, such as those developed based on the large-eddy simulation (LES) concept [1–5], can greatly help with the development and assessment of new combustion systems. However, despite their great potentials, LES models have not been fully used for this purpose for several reasons. One reason is the difficulty of modeling of subgrid-scale (SGS) correlations in complex flow configurations, which can significantly affect the accuracy of LES results. The modeling of SGS correlations is significantly more difficult in turbulent reacting flows particularly when the flow is compressible. This is not just due to the additional

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nonlinearity of chemical source or sink terms, but also due to the intricate complexities of turbulence-reaction interactions [6] and the presence of shock/detonation waves. Several books and reviews are available for the various SGS closures currently in use [1–5,7–11]. Some of the most promising models for LES of turbulent reacting flows are those developed based on the solution of the SGS probability density function (PDF), termed the filtered density function (FDF) [11–19]. In this approach, the joint statistics of turbulent variables at the subgrid level are obtained from the transport equation for the single-point joint FDFs of these variables. All terms involving single-point statistics appear in a closed form in the FDF equation, regardless of their complexity. This is the main advantage of the FDF method. However, the single-point FDF equation is not closed, and some form of modeling for multipoint correlations is needed.

Jaberi et al. [14] were the first to develop a FDF model for LES of variable density turbulent reacting flows based on the scalar filtered mass density function (FMDF), which is essentially the mass weighted filtered value of the fine-grained densities of energy and species mass fractions. This model was extended to the velocity-scalar [20,21] and velocity-scalar-frequency FMDF [22] later on. The scalar FMDF has been applied to a variety of combustion problems [23–30]. However, in the previous applications of the LES/FMDF, the effect of pressure on the scalar FMDF or the velocity-scalar-frequency FMDF was not considered. This effect could be ignored at low-Mach-number flows or constant pressure combustion. However, it should be included in the FMDF for high-speed subsonic or supersonic flows. Compressibility effects can be implemented in both scalar and velocity-scalar-frequency formulations of the FMDF. In the second formulation, the pressure and energy variables are directly included in the FMDF. However, in the first formulation, the FMDF involves the temperature and not the pressure. In this formulation, the compressibility terms are included via source terms added to the energy equation. The first formulation of the FMDF is much more manageable computationally, and the second one is more rigorous from the mathematical/statistical standpoint. At this time, the scalar FMDF model is the only practical formulation of FMDF for high-speed turbulent reacting flows. The energy-pressure-velocity-scalar-frequency formulation of the FMDF is currently under development [31]. The main objective of this work is to extend the scalar FMDF model to compressible flows. This is accomplished by adding a source term, obtained from the filtered velocity and pressure fields, to the FMDF equation. Three different subsonic and supersonic flows are simulated with the new compressible scalar FMDF model and its efficient numerical method. The first simulated flow involves the compression of a gas in a simple piston-cylinder assembly, called the rapid compression machine (RCM). The second flow is that in a three-dimensional shock tube, and the third flow is a supersonic coaxial helium–air jet. For the last flow, the velocity and scalar fields, as computed by the LES/FMDF with different SGS stress models, are compared with the experiment. The LES/FMDF results shown in Sec. III show that the pressure variations and compressibility effects are important in all these flows. They also show that the new compressible scalar FMDF model is able to capture the main features of these flows with reasonable accuracy.

II. Governing Equations

In the hybrid LES/FMDF methodology, two sets of Eulerian and Lagrangian equations are solved together for the velocity, pressure, and scalar (temperature and mass fraction) fields. These equations are presented and discussed in the following sections.

A. Filtered Compressible Navier–Stokes Equations

The standard filtered compressible mass, momentum, and energy equations in curvilinear coordinate systems can be written in the following compact form [28,32,33]:

\[
\begin{aligned}
\frac{\partial (\rho U)}{\partial \tau} + \frac{\partial (\rho \hat{U} - F_{\xi})}{\partial \xi} + \frac{\partial (\rho \hat{V} - G_{\eta})}{\partial \eta} + \frac{\partial (\rho \hat{W} - H_{\zeta})}{\partial \zeta} &= JS_{\rho} \\
J &= \delta(x, y, z, t)/\delta(\xi, \eta, \zeta, t) \text{ the Jacobian of transformation,} \\
U &= (\rho, \rho \hat{u}, \rho \hat{v}, \rho \hat{w}, \rho \hat{E}) \text{ is the solution vector. The inviscid fluxes in Eq. (1), } F, G, \text{ and } H \text{ are defined as}
\end{aligned}
\]

where \( J = \delta(x, y, z, t)/\delta(\xi, \eta, \zeta, t) \) is the Jacobian of transformation, and \( U = (\rho, \rho \hat{u}, \rho \hat{v}, \rho \hat{w}, \rho \hat{E}) \) is the solution vector. The inviscid fluxes in Eq. (1), \( F, G, \) and \( H \) are defined as

\[
\begin{aligned}
F &= \begin{bmatrix}
\rho \hat{U} \\
\rho \hat{u} \hat{U} + \rho \hat{E}_{\xi} \\
\rho \hat{u} \hat{V} + \rho \hat{E}_{\eta} \\
\rho \hat{u} \hat{W} + \rho \hat{E}_{\zeta} \\
(\rho \hat{E} + \rho \hat{U} - \hat{E}_{\xi})
\end{bmatrix}, \\
G &= \begin{bmatrix}
\rho \hat{V} \\
\rho \hat{v} \hat{V} + \rho \hat{E}_{\eta} \\
\rho \hat{v} \hat{W} + \rho \hat{E}_{\zeta} \\
(\rho \hat{E} + \rho \hat{V} - \hat{E}_{\eta})
\end{bmatrix}, \\
H &= \begin{bmatrix}
\rho \hat{W} \\
\rho \hat{w} \hat{W} + \rho \hat{E}_{\zeta} \\
(\rho \hat{E} + \rho \hat{W} - \hat{E}_{\zeta})
\end{bmatrix}
\end{aligned}
\]

with \( \hat{E}_{\xi} = J\partial \hat{E}/\partial \xi, \hat{E}_{\eta} = J\partial \hat{E}/\partial \eta, \text{ etc.} \), being the metric coefficients [32]. The definitions for viscous fluxes in curvilinear coordinate systems \( \hat{F}, \hat{G}, \) and \( \hat{H} \) are given in [28]. For a single-phase reacting flow, the source term vector in the right-hand side (RHS) of Eq. (1) is \( S_{\rho} = (0, 0, 0, 0, \hat{Q}) \).

For compressible flows, different forms of the “energy” equation may be solved. Here, we solve the equation for the total filtered energy based on the internal energy, \( \hat{E} = \hat{e} + (1/2)\hat{u} \hat{u} \). The convection of the SGS kinetic energy by the SGS velocity is ignored. However, the subgrid stress terms in Eq. (1) are modeled by a gradient-type closure. In this closure, the effective viscosity \( \mu_{e} = \mu + \rho \hat{v}_{l} \) is a function of the molecular viscosity and the turbulent kinetic viscosity \( \nu_{l} \). The latter is modeled by the Smagorinsky or modified kinetic energy (MKEV) closures. The turbulent kinetic viscosity in the Smagorinsky closure is \( \nu_{l} = (C_{m} \Delta_{k})^{2} \hat{S} \), and in the MKEV closure is \( \nu_{l} = C_{m} \Delta_{k} \sqrt{\hat{u}^{2} \hat{u}^{2} - (\hat{u}^{2})_{l}} / (\hat{u}^{2})_{l} \), where \( \Delta_{k} = (\nu_{l} / \nu_{e})^{1/3} \) is the characteristic size of the filter function and \( \nu_{e} = \hat{u}_{l} \hat{u}_{l} \). (\( \nu_{e} \) denotes the secondary filter function, and \( \nu_{e} / \nu_{e} = \nu_{e} \) is added to ensure the Galilean invariance of the model). The SGS velocity-energy and velocity-pressure correlations in the total filtered energy equation are also modeled with gradient-type closures [34,35].

The discretization procedure of the carrier fluid is based on the fourth-order compact finite difference (FD) scheme [36]. The “spectral nature” of compact differencing makes it suitable for LES. However, compact schemes cause significant numerical oscillations when there are discontinuities like shock waves in the flow. Cook et al. [37–39] introduced high-wave-number artificial viscosity/ conductivity to remove some of the numerical oscillations of the compact scheme. An extended version of the artificial viscosity/ conductivity was developed later on by Fiorina and Lele [40] and Kawai and Lele [41] for curvilinear grids, which is adopted in this work. Only low-Mach-number supersonic flows are considered.

B. Compressible Scalar Filtered Mass Density Function Equations

The scalar FMDF represents the joint PDF of the scalar PDF at the subgrid-level and is defined as

\[
P_{\phi} (\Psi; x, t) = \int_{-\infty}^{\infty} \rho(x', t) \sigma(\Psi, \Phi(x', t)) G(x' - x) \, dx'
\]

\[
\sigma(\Psi, \Phi(x, t)) = \prod_{n=1}^{N} \delta(\psi_{\alpha} - \phi_{\alpha}(x, t))
\]

where \( G \) denotes the filter function, \( \Psi \) is the scalar variable in the sample space, and \( \sigma \) is the “fine-grained” density [13]. The fine-grained density, as defined in Eq. (4), is the product of a series of delta functions. The scalar vector \( \Phi = \phi_{\alpha} \) (\( \alpha = 1, \ldots, N_{s} + 1 \)) includes...
the species mass fractions and the specific enthalpy. The scalar
FMDF transport equation is obtained from the transport equation for the
unfiltered scalar:
\[
\frac{\partial \rho \phi_\alpha}{\partial t} + \frac{\partial \rho u_i \phi_\alpha}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\Gamma \frac{\partial \phi_\alpha}{\partial x_i}\right) + \rho\left(S_{\alpha}^g + S_{\alpha}^{mop}\right)
\] (5)

Here, for simplicity, we consider the scalar equation in the Cartesian
cordinate system. For the species mass fraction \[\alpha = 1, \ldots, N_s\], the source/sink term \(S_{\alpha}^g\) is \(\dot{\bar{w}}_\alpha\). In Eq. (5) represents the production or consumption of species \(\alpha\) due to reaction. For the energy or enthalpy \([\alpha = N_s + 1]\), the source term \(S_{\alpha}^g = \dot{\bar{Q}}\) represents the heat of combustion, and the term \(S_{\alpha}^{mop} = (1/\rho)(\partial p/\partial t) + u_i (\partial p/\partial x_i) + \tau_{ij}(\partial u_i / \partial x_j)\) is due to compressibility and viscous
energy dissipation. The FMDF transport equation is obtained by
inserting the instantaneous unfiltered scalar equation [Eq. (5)] into the
time derivative of fine-grained density \((\partial \rho_\alpha / \partial t) = -(\partial \rho / \partial t)(\partial \rho_\alpha / \partial \rho))\), and, filtering that,
\[
\frac{\partial P_L}{\partial t} + \frac{\partial}{\partial x_i}\left(\rho u_i P_L\right) = -\frac{\partial}{\partial x_i}\left[\left(\frac{1}{\rho} \frac{\partial \rho}{\partial x_i} \Gamma \frac{\partial \phi_\alpha}{\partial x_i}\right) \Psi\right] P_L + \frac{\partial}{\partial \psi_\alpha}\left(\left[S_{\alpha}^{mop}\right] \Psi\right) P_L
\] (6)

\(S_{\alpha}^g = \dot{\bar{w}}_\alpha\) and \(S_{\alpha}^{mop} = 0\) \[\alpha = 1, \ldots, N_s\]
\(S_{\alpha}^g = \dot{\bar{Q}}\) and \(S_{\alpha}^{mop} = (1/\rho) (\rho_\alpha \partial u_i / \partial x_i + \rho \partial u_i / \partial x_j + \tau_{ij}(\partial u_i / \partial x_j))\) \[\alpha = N_s + 1\]

Equation (6) is an exact transport equation for the scalar FMDF in
compressible flows. In this equation, the Lewis number is assumed to
be unity, so the mass and thermal diffusion coefficients will be
similarly obtained from the viscosity as \(\nu = \mu / Sc\). The conditional
filtered terms involving \(S_{\alpha}^g\) and \(S_{\alpha}^{mop}\) represent the effects of chemical
reaction, viscous dissipation, and pressure on the FMDF. The second
term on the RHS of Eq. (6) is the chemical reaction term, which is
closed \((\left[S_{\alpha}^g\right] \Psi = S_{\alpha}^g(\Psi)\) when the effect of SGS pressure
fluctuations are ignored. With this assumption, the density in the
FMDF is approximated as \(\rho = \rho(\phi_\alpha, (\rho))\). The FMDF equation cannot be solved directly due to the presence of three unclosed terms.
The first one is the convection term [the second term on the LHS of
Eq. (6)], which can be decomposed into large-scale convection by the
filtered velocity and the SGS convection as [14]
\[
\langle u_i(\Psi)\rangle P_L = \langle u_i(\nu)\rangle P_L + \langle u_i(\Psi)\rangle P_L - \langle u_i(\nu)\rangle P_L
\] (7)
The SGS convection is modeled here with a gradient-type closure:
\[
\langle u_i(\Psi)\rangle P_L = \langle u_i(\nu)\rangle P_L - \Gamma_i \frac{\partial (P_L / \rho)}{\partial x_i}
\] (8)
where \(\Gamma_i = (\rho \nu P_r) / P_r\) is the turbulent diffusivity and \(P_r\) is the
transport parameter (turbulent Prandtl and Schmidt numbers are the
same). This model is similar to the ones we used in our previous
works for low-Mach-number variable density flows. However, \(\nu_i\) is calculated with a compressible SGS model.

The second unclosed term in the FMDF transport equation [the
first term on the RHS of Eq. (6)] is also decomposed into two parts:
the molecular transport and the SGS mixing parts. The SGS mixing is
modeled with the linear mean-square estimation [42,43] model, also
known as interaction by exchange with the mean model [44]. Consequently, we have

\[
\frac{\partial}{\partial \psi_\alpha} \left[\left(\frac{1}{\rho} \frac{\partial \rho}{\partial x_i} \Gamma \frac{\partial \phi_\alpha}{\partial x_i}\right) \Psi\right] P_L = \frac{\partial}{\partial x_i}\left[\Gamma \left(\frac{\partial (P_L / \rho)}{\partial x_i}\right)\right] + \frac{\partial}{\partial \psi_\alpha}\left(\Omega_{\alpha}(\psi_\alpha - \langle \phi_\alpha \rangle) P_L\right)
\] (9)

The SGS mixing frequency, \(\Omega_{\alpha} = C_m(\Gamma + \Gamma_r)/\Delta_{\alpha}^2(\rho)\) in
Eq. (9), is obtained from the molecular and turbulent SGS diffusivities
\((\Gamma + \Gamma_r)\) and the filter length \(\Delta_{\alpha}\).

To extend the Reynolds-averaged Navier–Stokes (RANS) PDF method to compressible flows, Delarue and Pope [45] considered the
pressure as one of the random variables in the PDF formulation and
solved a set of modeled stochastic equations for the joint velocity-
frequency-energy-pressure PDF. In the scalar FMDF model
considered in this study, the pressure is not directly included in the
FMDF formulation, and only the effect of filtered pressure on the
scalar FMDF is considered. The last term on the RHS of Eq. (6)
represents the effect of pressure and viscosity on the scalar FMDF.
Here, the temporal derivative of pressure in that term is approximated as

\[
\left(\frac{1}{\rho} \frac{\partial (P_L / \rho)}{\partial t}\right) \Psi\right] P_L = \frac{1}{\langle \rho \rangle} \left(P_L / \langle \rho \rangle\right) P_L \quad \alpha = N_{s+1}
\] (10)

and the spatial derivative is decomposed into the filtered and SGS parts:

\[
\left(\frac{1}{\rho} \frac{\partial (P_L / \rho)}{\partial \xi}\right) \Psi\right] P_L = \frac{1}{\langle \rho \rangle} \left(P_L / \langle \rho \rangle\right) P_L + \left(\frac{(1/\rho) \partial (P_L / \rho)}{\partial \xi}\right) P_L
\] (11)

Similarly, the viscous dissipation effect on the scalar FMDF is
decomposed into the resolved and SGS parts:

\[
\left(\frac{1}{\rho} \frac{\partial (\nu)}{\partial \xi}\right) \Psi\right] P_L = \frac{1}{\langle \rho \rangle} \left(P_L / \langle \rho \rangle\right) \left(\frac{(1/\rho) \partial (\nu)}{\partial \xi}\right) P_L + \left(\frac{(1/\rho) \partial (\nu)}{\partial \xi}\right) P_L
\] (12)

The effects of SGS pressure and viscous dissipation on the scalar
field may become significant in high-speed flows. A comprehensive
study of these effects requires detailed direct numerical simulation
and experimental data for these flows. In this study, we ignore the
SGS viscous term in Eq. (12) and the SGS pressure term in Eq. (11).
By inserting Eqs. (7–12) into Eq. (6), the final form of the FMDF
transport equation for a compressible reacting system becomes

\[
\frac{\partial P_L}{\partial t} + \frac{\partial (\langle u_i \rangle P_L)}{\partial x_i} = \frac{\partial}{\partial x_i}\left[\left(\Gamma + \Gamma_r\right) \frac{\partial (P_L / \rho)}{\partial x_i}\right] + \frac{\partial}{\partial \psi_\alpha}\left(\Omega_{\alpha}(\psi_\alpha - \langle \phi_\alpha \rangle) P_L\right)
\] (13)

where

\[
\left\{ S_{\alpha}^g = \dot{\bar{w}}_\alpha\right. \text{and } \left. S_{\alpha}^{mop} = 0\right\} \quad \alpha = 1, \ldots, N_s
\]
\[S_{\alpha}^g = \dot{\bar{Q}}\] and \(S_{\alpha}^{mop} = (1/\rho)(\partial \rho / \partial x_i + \langle u_i \rangle P_r / \partial x_i + \langle \tau_{ij} \rangle P_r / \partial x_i)\) \[\alpha = N_{s+1}\]

Note that the repeated \(\alpha\) in Eq. (13) does not imply summation.
This is a modeled transport equation for the FMDF that can be solved by
a hybrid numerical method described in the next section.
Equation (13) can be integrated in the composition \(\Psi\) domain
to obtain the transport equations for the SGS moments. The equation
for the first SGS moment \(\langle \phi_1 \rangle\) is

\[
\frac{\partial (\phi_1)}{\partial t} + \frac{\partial (\langle u_1 \rangle \phi_1)}{\partial x_i} = \frac{\partial}{\partial x_i}\left[\left(\Gamma + \Gamma_r\right) \frac{\partial \langle \phi_1 \rangle}{\partial x_i}\right]
\]
This equation can also be obtained directly by filtering Eq. (5), using a standard gradient model for the subgrid flux terms and neglecting the SGS viscous and pressure terms.

C. Numerical Solution

In the modeled scalar FMDF equation [Eq. (13)], the velocity and pressure fields are not known and must be obtained by other means. Here, the filtered velocity and pressure are obtained by solving Eq. (1) with conventional FD methods. With the known filtered velocity and pressure fields, the modeled FMDF equation can be solved by the Lagrangian Monte Carlo (MC) procedure [46]. In this procedure, each MC particle undergoes motion in physical space due to filtered velocity and molecular and subgrid diffusivities. The particle motion represents the spatial transport of the FMDF and is modeled by the following stochastic differential equation (SDE) [47]:

\[ \text{d}X^\alpha = \left[ \langle u^\alpha \rangle_L + \frac{1}{\langle \rho \rangle_L} \frac{\partial (\Gamma + \Gamma^f)}{\partial x^i} \right] \text{d}t + \left[ \sqrt{2(\Gamma + \Gamma^f)} \frac{1}{\langle \rho \rangle_L} \right] \text{d}W^i \]

(15)

where \( W^i \) denotes the Wiener process [48]. The scalar value of each particle is changed due to mixing, reaction, viscous dissipation, and pressure variations in time and space. The change in scalar space is described by the following SDEs:

\[ \text{d}\phi^\alpha = -\Omega_{\alpha \beta} (\phi^\beta - \langle \phi^\beta \rangle_L) \text{d}t + (S_{\alpha \beta}^g + S_{\alpha \beta}^{mp}) \text{d}t \]

(16)

When combined, the diffusion processes described by Eqs. (15) and (16) have a corresponding Fokker–Planck equation that is identical to the FMDF transport equation [Eq. (13)].

To reduce the number of MC particles and the computational cost, a procedure involving the use of nonuniform weights is also considered. This procedure allows a smaller number of particles in regions in which a low degree of variability is expected. Conversely, in regions of high variability, a large number of particles is allowed. The particle weighting of particles allows the particle number density to stay above a certain minimum number [46]. To calculate the Favre-filtered values of any variable at a given point, MC particles are weighted averaged over a box of size \( \Delta_E \) centered at the point of interest [14]. The Favre-filtered value of any function of scalars, like \( Q(\phi) \), is obtained from the following weighted averaging operation:

\[ \langle Q \rangle_L \approx \frac{\sum_{n \in \Delta_E} w^{(n)} Q(\phi)}{\sum_{n \in \Delta_E} w^{(n)}} \]

(17)

where \( w^{(n)} \) represents the weight of a MC particle within the ensemble domain \( \Delta_E \). It has been shown [14,46] that the sum of weights within the \( \Delta_E \) is proportional to the filtered fluid density as

\[ \langle \rho \rangle_L \approx \frac{\Delta m}{V_E} \sum_{n \in \Delta_E} w^{(n)} \]

(18)

where \( V_E \) is the volume of the domain and \( \Delta m \) is the mass of each MC particle with a unit weight. Using Eq. (17), one can calculate the fluid density from the MC particles as

\[ \langle \rho \rangle L \approx \left( \frac{\sum_{n \in \Delta_E} w^{(n)} (RT \langle \rho \rangle)_{L}}{\sum_{n \in \Delta_E} w^{(n)}} \right)^{-1} \]

(19)

The computed filtered density from the MC particles [Eq. (19)] should be the same as the filtered fluid density obtained from Eq. (1) and the weighted particle number density calculated by Eq. (18).

To include the compressibility in the FMDF formulation, the total derivative of filtered pressure, as computed by the filtered Eulerian carrier-gas equations, is interpolated and added to the corresponding MC particles. Artificial viscosity causes the primitive variables to become smooth across the flow discontinuities. However, the

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Fig. 1 Elements of the hybrid LES/FMDF mathematical and computational methodology: a) diagram showing coupling between LES-FD and FMDF-MC parts and b) computational domain and grid.
computed derivatives of these variables may still be noisy, causing the FMDF values to become inaccurate and unphysical. To solve this problem, a flux limiter scheme is used. The main idea behind the flux limiter scheme is to limit the spatial derivatives of flow variables to realizable values. Here, van Leer’s one-parameter family of the minmod limiters [49] is used to calculate the spatial derivative of the filtered pressure $\tilde{p}$:

$$\frac{\partial \tilde{p}}{\partial x_i} = \minmod \left( \theta \frac{\tilde{p}_{i+1} - \tilde{p}_{i}}{\Delta x}, \frac{\tilde{p}_{i+1} - \tilde{p}_{i-1}}{2\Delta x}, \theta \frac{\tilde{p}_{i+1} - \tilde{p}_{i}}{\Delta x} \right)$$

(20)

where $\theta \in [1, 2]$ and the multivariable minmod function is defined as

$$\minmod (a_1, a_2, \ldots) = \begin{cases} \min[a_i] & \text{if } a_i > 0 \forall i \\ \max[a_i] & \text{if } a_i < 0 \forall i \\ 0 & \text{otherwise} \end{cases}$$

In the original version of this limiter [49], the minmod value of derivatives is calculated with a second-order central, a first-order forward, and a first-order backward differencing. In this work, instead of a second-order central differencing scheme, the fourth-order compact differencing is employed. In addition to the pressure, the spatial derivatives of turbulent diffusion coefficient $\Gamma_p$, as required in Eq. (15), are calculated by the van Leer limiter to avoid unphysical particle movements across the shock.

Figure 1a shows some of the main features of our hybrid compressible LES/FMDF methodology. For the solution of filtered Eulerian carrier-gas equations [Eq. (1)], any high-order numerical method may be used. As described before, the discretization procedure for this equation in this work is based on the fourth-order compact FD scheme and third-order low-storage Runge–Kutta method. The FD equations are solved with “standard” closures for the SGS stress and scalar flux terms and the artificial viscosity. The SDEs are solved with the MC procedure. The filtered velocity and the derivatives of filtered pressure and velocity are computed over the FD grid points and then interpolated from the FD grid points to the MC particle locations. Figure 1b shows the FD grid points, some of the MC particles, and a sample ensemble domain used for the particle averaging. In the present hybrid methodology, the filtered values of variables like temperature can be calculated from the LES-FD and FMDF-MC data. This provides a unique opportunity for the assessment of FD and MC methods, because consistency of MC and FD data implies the numerical accuracy of both methods. For establishing the consistency of FD and MC methods in reacting flows, the chemical terms that are closed in the FMDF-MC formulation are calculated from MC particles and used in the FD equations.

III. Results

To test the new compressible scalar FMDF model, the scalar mixing and heat transfer in three different flows are considered. As shown next, the compressibility effect is important in all three flows.

A. Rapid Compression Machine

The first flow considered in this paper is an isotropic turbulent flow going through compression in a simple piston-cylinder assembly, called the RCM. The goal of conducting the RCM simulations is to study the pressure effect on the FMDF in a compressible but subsonic flow. The experimental setup for the Michigan State University (MSU) RCM [50] is somewhat similar to that considered in [51] and is shown in Fig. 2a. The geometry is axisymmetric and consists of a simple closed cylinder and a flat piston. The compression ratio in the RCM is around 21. To avoid a grid singularity at the centerline, a rectangular H-H (250 $\times$ 13 $\times$ 13) block was employed at the center, coupled with an O-H (250 $\times$ 45 $\times$ 42) grid outside. Figure 2b shows the three-dimensional and two-dimensional views of the grid. The geometrical parameters and piston movement are similar to those used in the MSU RCM experiment, although the exact shape of the piston is different. During the gas compression, the grid cells are nonuniformly compressed, although their number is not changed. The initial velocity field at the beginning of compression is an isotropic turbulent flow obtained by direct numerical simulation of the Navier–Stokes equations with periodic boundary conditions. The initial temperature is assumed to be uniform at 300 K with no perturbation. The initial pressure is also uniform at atmospheric throughout the cylinder. The initial turbulent intensity is estimated to be around 10% of the mean piston speed (8.5 m/s). The walls are assumed to be adiabatic.

To include the pressure effect in the scalar FMDF model, the derivative of filtered pressure $D(\bar{p})/Dt$, as computed from the FD data are interpolated and added to the corresponding MC particles. Consistency of the filtered temperatures obtained by the Lagrangian MC method with those calculated by the FD solution of Eulerian equations is dependent on the inclusion of $D(\bar{p})/Dt$ in the FMDF equation. This is clearly demonstrated in Fig. 3a, in which the spatial variations of the gas temperature along the cylinder centerline at different piston locations (locations 1 to 5 in Fig. 3b) or different

![Fig. 2](image-url)
times are shown. In this figure, solid lines, square symbols, and dotted lines with delta symbols represent FD, MC with \(D_{hp} = D_t\), and MC without \(D_{hp} = D_t\) results, respectively. A comparison between MC results obtained with and without \(D_{hp} = D_t\) indicate the critical role of pressure in the FMDF equation during the compression in the RCM. There seems to be a good consistency between the FD and MC results when \(D_{hp} = D_t\) is included in the FMDF equation. It should be mentioned that, because the flow in the RCM is low-Mach number, the term \(\partial p/\partial t\) in the enthalpy equation is small and can be ignored, i.e., \(D(p)/Dt \approx \partial(p)/\partial t\).

**B. Shock Tube**

The second flow considered in this paper is an isotropic turbulent flow interacting with a shock wave in a shock “tube.” The initial condition for the thermodynamic variables is based on Sod’s shock tube solution [52] with initial pressure ratio of \(p_i/p_f = 10\) and density ratio of \(\rho_i/\rho_f = 8\). However, unlike the Sod’s problem, the initial flow is an isotropic turbulent flow (similar to that in the RCM) with intensity of 6% of the laminar shock upstream velocity, which is about 450 m/s. The turbulent Mach number in the low-pressure zone of the flow is about 0.054. The preceding shock tube problem was simulated with the LES/FMDF model in a rectangular domain with a three-dimensional \(\text{H-H} (380 \times 64 \times 64)\) grid. Wall boundary conditions are used for the first and last points in the axial direction, but the flow is assumed to be homogeneous and periodic in the other two directions for simplicity. For the FMDF solution, the MC particles are randomly distributed in the computational domain based on the initial condition. To assess the performance of the artificial viscosity, two sets of laminar simulations are also performed with and without artificial viscosity. In Figs. 4a and 4b, the pressure and velocity as predicted by the compact differencing without artificial viscosity, \(\mu^*\) denotes the artificial viscosity: a) pressures and b) velocities.

**Fig. 3** RCM: a) temperatures obtained from the FD and MC data at different piston locations during the compression in the RCM and b) different piston locations during the compression.

**Fig. 4** Comparison of pressures and velocities obtained by the FD with artificial viscosity (solid lines with solid triangular symbols) and without artificial viscosity (solid lines with hollow triangular symbols) with the analytical solutions (solid lines no symbol) for Sod’s shock tube problem; \(\mu^*\) denotes the artificial viscosity: a) pressures and b) velocities.

**Fig. 5** Comparison of temperatures obtained by the FD, MC without \(D_{hp} = D_t\), MC with \(\partial p/\partial t\), MC with limiter on \(D_{hp} = D_t\), for the Sod shock tube problem.
viscosity at $t = 0.2$ are compared with those obtained by the compact differencing with artificial viscosity. The analytical solution is for the one-dimensional inviscid shock tube problem. Figure 4 shows that the numerical oscillations in the flow decreases when the artificial viscosity is added.

The FMDF-MC temperatures obtained with different pressure models in the shock tube with turbulence is compared with the LES-FD temperatures in Fig. 5. In this figure, the dash-dotted line with the diamond symbols represents the FMDF results without the pressure term $D(p)/Dt$. Without this term, MC particles can not correctly predict the gas temperature in the vicinity of the shock wave, the contact surface and the expansion waves. The FMDF temperatures with $\partial(p)/\partial t$ are showing a better consistency with the FD temperatures. However, a good consistency between LES-FD and FMDF-MC results is not achieved with just the $\partial(p)/\partial t$ term because the $\langle u \rangle, \partial(p)/\partial x,$ term is also important for high-Mach-number flows. This is demonstrated in Fig. 5, in which it is shown that the MC results are fully consistent with the FD results when $D(p)/Dt$ term, calculated with the van Leer limiter, is added to the MC particles. Without the limiter, the spatial derivative of pressure has some unphysical oscillations, which lead to the underprediction of MC temperature.

The isolevels of instantaneous filtered temperature as obtained by the LES-FD and FMDF-MC are shown in Figs. 6a and 6b, respectively. Evidently, the shock wave has a significant effect on the turbulence. Nevertheless, the LES-FD and FMDF-FD predictions

![Fig. 6 Instantaneous isolevels of the filtered temperature predicted by a) LES-FD and b) FMDF-MC in Sod’s shock tube.](image)

![Fig. 7 Companion of FD and MC filtered densities calculated by Eqs. (1) and (19) with the weighted MC particles number density calculated by Eq. (18) in the shock tube: a) 6 MC particles per cell, b) 24 MC particles per cell, c) 48 MC particles per cell, and d) companion of FD and MC densities.](image)
are shown to be consistent, even in the vicinity of the shock wave, which indicates that the compressible scalar FMDF model is able to capture the shock wave effects on the turbulence.

Figure 7 shows the fluid densities and the weighted MC particle number densities for the simulations started with 6, 24, and 48 initial particles per cell. As mentioned in Sec. II.C, the filtered fluid density [calculated from the MC particles via Eq. (19)] and the weighted MC particle number density [calculated by Eq. (18)] should be equal to the filtered fluid density (calculated from the FD data). Oscillatory results for the weighted MC particle number density are expected, as they are obtained by averaging of Lagrangian particles’ weight within each cell. However, by increasing the initial number of MC particles, the predicted particle number density shows less oscillations and converges to the filtered fluid density. This indicates the correct transport of MC particles, even in the presence of a strong shock wave. In Fig. 7d, the filtered density calculated from the MC particles is compared with those obtained from the FD data. The numerical results are shown to be close to the analytical one-dimensional inviscid solution, even though the simulations are three-dimensional, turbulent and viscous. Initially only six MC particles per cell are employed for the FMDF solution, yet the computed FMDF-MC densities compare very well with LES-FD densities at later times. The oscillations in the weighted MC particle number density seem to have a negligible effect on the filtered variables calculated from the MC particles. In fact, we found the FMDF-MC predictions of the filtered density and temperature to be always consistent with the LES-FD predictions for all tested particle/flow conditions at all times.

C. Coaxial Helium–Air Jet

The third flow configuration considered in this paper is a supersonic coaxial helium–air jet (Fig. 8a). The geometry is axisymmetric and consists of a central and an outer concentric annular nozzle passage. The thickness of the central nozzle at the flow outlet is 0.5 mm. This flow has been studied experimentally and numerically with RANS models [53,54]. LES of this flow on a Cartesian grid is also reported [31,55]. Here, we have simulated the flow with the LES-FD model, using a six-block grid and the compressible FMDF model. Figure 8b shows the three-dimensional and two-dimensional views of the grid we used in our LES/FMDF calculations. Similar to the grid used for the RCM simulation, the coannular grid has a rectangular H-H block in the center for avoiding the polar singularity. Three different grid resolutions are employed (see Table 1 for more details). In grid G2, the resolution in the inner jet region (x < 270 mm) along the axial direction is about twice of that in grid G1. In grid G3, the radial grid resolution in the entire domain is twice of that in grid G1. The gas mass fraction at the central-nozzle inlet is 0.7039 for the helium (He) and 0.2961 for the oxygen (O2). The total pressure and density are 628.3 kPa and 1.334 kg/m³, respectively. The outer coflow is air with a total pressure and density of 580.0 kPa and 6.735 kg/m³, respectively. At the nozzles’ inlet, the values of pressure and density are fixed according to experimental values, and it is assumed that the inlet flows are always parallel to the walls. The computed velocity components at the nozzles’ outlet are used as inlet conditions for the jet flow simulations with an added random perturbation [56–58] with an amplitude of 3% of nozzles’ outlet maximum axial velocity. For

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**Table 1** Three O-H (x, r, θ) grids employed for the coaxial helium–air jet simulations; for the central region, a 13 × 13 (y, z) H-H grid is used

<table>
<thead>
<tr>
<th>Grid</th>
<th>Inner nozzle</th>
<th>Outer nozzle</th>
<th>Jet</th>
<th>Ambient</th>
<th>Cells × 10⁶</th>
</tr>
</thead>
<tbody>
<tr>
<td>G1</td>
<td>126 × 28 × 42</td>
<td>126 × 56 × 42</td>
<td>172 × 92 × 42</td>
<td>196 × 56 × 42</td>
<td>1.6</td>
</tr>
<tr>
<td>G2</td>
<td>126 × 28 × 42</td>
<td>126 × 56 × 42</td>
<td>282 × 92 × 42</td>
<td>306 × 56 × 42</td>
<td>2.3</td>
</tr>
<tr>
<td>G3</td>
<td>126 × 55 × 42</td>
<td>126 × 111 × 42</td>
<td>172 × 182 × 42</td>
<td>196 × 110 × 42</td>
<td>3.2</td>
</tr>
</tbody>
</table>
the outlet boundary, a characteristic boundary condition with extrapolation is used. The time step is updated every time step based on the Courant–Friedrichs–Lewy condition. The average time step for this problem is about $1.5 \times 10^{-8}$ s. The passover time is calculated with the averaged velocities of the inner and outer jets ($800 \text{ m/s}$) and is $7.5 \times 10^{-4}$ s. Before gathering and averaging the data, the flow is simulated for about four passover times. The LES/FMDF calculations were performed with the Smagorinsky model with constant coefficient of $C_D = 0.1$ and with the MKEV model with constant coefficients of $C_m = 0.02, 0.025, \text{ and } 0.03$ are employed. The predicted time-averaged axial velocity with different MKEV model constants are compared with the experimental data at four jet locations in Fig. 10a. These simulations are all using grid G1. The MKEV model predictions with all three model coefficients are in agreement with the experiment. However, the LES predictions with $C_m = 0.03$ are found to be the closest to the experimental data.

Figure 10b shows the time-averaged values of the axial velocity, calculated with the MKEV model with $C_m = 0.03$ and three different grids G1, G2, and G3. The higher-resolution results obtained with grids G2 and G3 are found to be close to the ones shown in Fig. 10b for the lower-resolution grid G1. Comparison of time-averaged axial velocity at different locations from the central nozzle with the experimental data in Fig. 11 again indicates that the LES with the MKEV model is able to accurately predict the experimental data. However, the predicted rms values of axial velocity in Fig. 12 show some deviation from the experiment for both models, even though the MKEV model predictions are much closer to the experimental data. The differences in rms values may be attributed to insufficient
For the coannular jet, the scalar statistics are calculated from both FMDF-MC and LES-FD data, with the pressure and viscous dissipation terms included in the FMDF equation. Contours of the instantaneous filtered temperature as obtained from the FD and MC data are shown in Figs. 13a and 13b, respectively. Qualitatively, LES-FD and FMDF-FD results are consistent. To better assess the pressure effect on the FMDF and the consistency of MC and FD results, the local values of temperature predicted by the FMDF-MC with and without the pressure term \( D_h p_i = D_t \) are compared with those of the LES-FD in Figs. 14b and 14c. In the low-temperature regions, the correlation coefficient is \( R = 0.74 \) when the pressure term \( D_h p_i = D_t \) term is ignored. However, the correlation coefficient increases to \( R = 0.97 \) by adding the \( D(p)_i / D_t \) term to the FMDF equation. In Fig. 15, the volume averaged values of the filtered temperature, conditioned on \( \langle u_i \rangle L \delta (p)_i / \delta x_i \) and calculated by the FMDF-MC with and without \( D(p)_i / D_t \) are compared with those of the LES-FD for different \( \langle u_i \rangle L \delta (p)_i / \delta x_i \) values. Evidently, the conditional LES-FD temperatures are consistent with the conditional FMDF-MC temperatures only when the \( D(p)_i / D_t \) term is included in the FMDF formulation.

Consistent with the results shown in Figs. 11 and 12 for the mean and rms of axial velocity, the LES predictions with the Smagorinsky model with \( C_d = 0.1 \) are not accurate for the simulated supersonic jet flow, but the MKEV predictions are in good agreement with the experimental data. This is demonstrated in Fig. 16, in which the time-averaged profiles of the He – O\(_2\) mass fraction are shown. Figure 16

grid resolution at the edge of separated plate or to the SGS models or to the uncertainty in the experimental measurements [54]. For the coannular jet, the scalar statistics are calculated from both FMDF-MC and LES-FD data, with the pressure and viscous dissipation terms included in the FMDF equation. Contours of the instantaneous filtered temperature as obtained from the FD and MC data are shown in Figs. 13a and 13b, respectively. Qualitatively, LES-FD and FMDF-FD results are consistent. To better assess the pressure effect on the FMDF and the consistency of MC and FD results, the local values of temperature predicted by the FMDF-MC with and without the pressure term \( D_h p_i = D_t \) are compared with those of the LES-FD in Figs. 14b and 14c. In the low-temperature regions, the correlation coefficient is \( R = 0.74 \) when the pressure term \( D_h p_i = D_t \) term is ignored. However, the correlation coefficient increases to \( R = 0.97 \) by adding the \( D(p)_i / D_t \) term to the FMDF equation. In Fig. 15, the volume averaged values of the filtered temperature, conditioned on \( \langle u_i \rangle L \delta (p)_i / \delta x_i \) and calculated by the FMDF-MC with and without \( D(p)_i / D_t \) are compared with those of the LES-FD for different \( \langle u_i \rangle L \delta (p)_i / \delta x_i \) values. Evidently, the conditional LES-FD temperatures are consistent with the conditional FMDF-MC temperatures only when the \( D(p)_i / D_t \) term is included in the FMDF formulation.

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also confirms that the FMDF-MC and LES-FD results are consistent with each other at different spatial locations throughout the flow. The time-averaged values of temperature in Fig. 17, like those shown in Fig. 16c for the He$/$O2 mass fraction, indicate that the LES-FD and FMDF-MC predictions are consistent. The computed rms of the resolved He$/$O2 mass fraction and temperature by the FMDF-MC and LES-FD in Figs. 18a and 18b are also in good agreement with each other, further indicating the consistency and the reliability of the LES/FMDF model in supersonic turbulent flows.

IV. Conclusions

The scalar FMDF model is further extended and employed for LESs of compressible turbulent flows by including the effect of pressure in the FMDF transport equation. The new compressible scalar FMDF model is applied to three subsonic and supersonic problems: an isotropic turbulent flow going through compression in a piston-cylinder assembly, a three-dimensional shock tube, and a...
coaxial supersonic helium–air jet. For the piston-cylinder assembly and shock tube, the consistency of FD and MC parts of the hybrid LES/FMDF model is established by adding the total derivative of pressure to the FMDF equation. For the coaxial helium–air jet, LES with the MKEV SGS model was able to predict the experimental values of the velocity and scalar at different locations. The FMDF-MC predictions for the scalar mass fraction and temperature are shown to be also consistent with those of the LES-FD in this flow, further indicating the reliability and applicability of the compressible LES/FMDF model to high-speed turbulent flows. The compressible scalar FMDF model is only applied to nonreacting flows in this paper. Reacting results will be presented in future papers. To develop a more accurate SGS PDF model for LES of high-speed turbulent reacting flows, a more complete formulation of the FMDF based on the joint velocity-frequency-energy-pressure-scalar FMDF has to be considered. However, the scalar FMDF model is computationally much less demanding and is applicable to practical combustion systems.

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