FILTERED DENSITY FUNCTION FOR LARGE EDDY SIMULATION OF TURBULENT REACTING FLOWS ON UNSTRUCTURED MESHES

by

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A new computational filtered density function (FDF) methodology is developed for large eddy simulation (LES) of turbulent reacting flows on an unstructured mesh. The effect of chemical reactions in the transport equation of FDF appears in a closed form, whereas the effects of scalar mixing and convection within the subgrid are modeled. The FDF transport equation is solved numerically by a particle based Lagrangian Monte Carlo (MC) method. The base filtered transport equations on the unstructured mesh are solved by a finite-volume (FV) method. The consistency of the hybrid FV-MC solver and the realizability of the simulated results are demonstrated via LES of a temporally developing mixing layer. The overall performance of the model is appraised by comparison with direct numerical simulation (DNS) data. Subsequently, the unstructured FDF simulator is employed for predictions of two swirl stabilized non-premixed flames. These are low-swirl (SM1) and high-swirl (SMA2) methane flames. The simulated results are assessed via comparison with experimental data and show excellent agreements. Finally, the unstructured FDF solver is extended to conduct LES of a realistic swirl flame combustor. This is the PRECCINSTA experimental burner from the German Aerospace Center (DLR). The simulated data are analyzed by comparison of the Reynolds-averaged statistics with experimental data and show excellent agreements.

**Keywords:** Large eddy simulation, filtered density function, turbulence, reacting flows.
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1.0 INTRODUCTION

One of the most challenging issues in energy and environment research is associated with accurate prediction of turbulent reacting flows. The optimal means of capturing the detailed, unsteady physics of such flows, as it is now widely believed, is via large eddy simulation (LES).\(^3\) The challenge in LES is accurate and consistent modeling of the subgrid scale (SGS) quantities.\(^4\) The filtered density function (FDF) methodology; including its mass weighted form, the filtered mass density function (FMDF), has proven particularly effective for this purpose.\(^5\) The FDF is essentially the probability density function (PDF) of the SGS quantities. Therefore, it provides all the statistical information pertaining to these quantities.

In its \textit{stand-alone} form, the FDF must account for the joint statistics of all the relevant physical variables. The most sophisticated FDF closure available to-date is the frequency-velocity-scalar FMDF (FVS-FMDF),\(^6\) and a simpler version (VS-FMDF) which does not include the SGS frequency.\(^7,8\) Hydrodynamic closure in incompressible, non-reacting flows has been successfully achieved via the velocity-FDF (V-FDF),\(^9\) and the one which has been utilized the most, only considers the scalar field (S-FDF and S-FMDF). This was the most elementary form of FDF when it was first introduced.\(^10,11\) Since this original work, FDF has experienced widespread usage, and is now regarded as one of the most effective and popular means of LES worldwide. Some of the most noticeable contributions in FDF by others are in its basic implementation,\(^12-26\) fine-tuning of its sub-closures\(^27-29\) and its validation via laboratory experiments.\(^16,30-34\) Despite its popularity, a major challenge associated with FDF is its implementation in complex combustion devices. The geometry of such devices is not easily amenable to the framework of structured grids. Structured grids may also lack the required flexibility and robustness for handling domains with complicated boundaries,
or the grid cells may become too skewed and twisted, thus prohibiting an efficient numerical simulation. In all the previous contributions, FDF is simulated on structured grids. This is obviously not ideal for engineering applications. An unstructured grid concept is considered as one of the appropriate solutions to the problem of producing grids in regions with complex shapes. Unstructured grids have irregularly distributed nodes and their cells are not obliged to have any one standard shape. Besides, the connectivity of neighboring grid cells varies from point to point and is not subject to any restrictions.

The objective of this dissertation is to extend the FDF methodology to unstructured meshes and to provide results based on its implementation for LES of chemically reacting turbulent flows with complex chemistry and geometries. This is achieved by developing the necessary numerical tools required to implement FDF on unstructured grids. These include an efficient method to track particles and a novel method to evaluate particle statistics on unstructured meshes. The FDF implementation is done in the commercial CFD code ANSYS FLUENT.

1.1 SCOPE

This dissertation is organized as follows. In Chapter 2, the FDF implementation on unstructured grids is discussed. The work described in this chapter is published in the *Journal of Computational Physics*. In Chapter 3, the unstructured S-FMDF methodology is employed for LES of two swirl stabilized non-premixed flames. The work described in this chapter is accepted for publication in the *AIAA Journal*. In Chapter 4, the S-FMDF methodology is further extended and employed for LES of a realistic gas turbine combustor (the PRECCINSTA experimental burner) from the German Aerospace Center, (DLR). In Chapter 5, some final remarks regarding the FDF implementation on unstructured grids are presented, along with some suggestions for future research. A part of this dissertation was presented at the 49th AIAA Aerospace Sciences Meeting and was the subject of an invited talk at the 47th AIAA/ASME/SAE/ASEE Joint Propulsion Conference. It was also published in a recent invited tutorial book chapter.
2.0 FILTERED DENSITY FUNCTION SIMULATOR ON UNSTRUCTURED MESHES

In the work described in this chapter, a new computational filtered density function (FDF) methodology is developed for large eddy simulation (LES) of turbulent reacting flows on an unstructured mesh. In this methodology, the effects of unresolved scalar fluctuations are taken into account by considering the probability density function (PDF) of subgrid scale (SGS) scalar quantities. The effect of chemical reactions in the transport equation of FDF appears in a closed form whereas the effects of scalar mixing and convection within the subgrid are modeled. The FDF transport equation is solved numerically by a particle based Lagrangian Monte Carlo (MC) method. The base filtered transport equations on the unstructured mesh are solved by a finite-volume (FV) method. An efficient method of tracking particles on an unstructured mesh is outlined and a “basis function method” method to compute particle means is developed. The consistency of the hybrid FV-MC solver on the unstructured mesh and the realizability of the simulated results are demonstrated via LES of a temporally developing mixing layer. The overall performance of the model is appraised by comparison with direct numerical simulation (DNS) data.

2.1 FORMULATION

In a turbulent flow undergoing chemical reaction involving $N_s$ species, the primary transport variables are the density $\rho(x, t)$, the velocity vector $u_i(x, t) \ (i = 1, 2, 3)$, the pressure $p(x, t)$, the total specific enthalpy $h_s(x, t)$, and the species mass fractions $Y_\alpha(x, t) \ (\alpha = 1, 2, \ldots, N_s)$. The equations which govern the transport of these variables in space ($x_i$) ($i = 1, 2, 3$) and
time \( (t) \) are the continuity, momentum, conservation of enthalpy (energy) and species mass fraction equations:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0,
\]

\[
\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_j u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j},
\]

\[
\frac{\partial \rho \phi_\alpha}{\partial t} + \frac{\partial \rho u_j \phi_\alpha}{\partial x_j} = -\frac{\partial J_j^\alpha}{\partial x_j} + \rho S_\alpha, \quad \alpha = 1, 2, \ldots, N_s + 1.
\]

These equations are coupled with an appropriate equation of state. The chemical reaction source terms \( S_\alpha \equiv S_\alpha (\phi(x,t)) \) are functions of compositional scalars \( \phi \equiv [\phi_1, \phi_2, \ldots, \phi_{N_s+1}] \) where \( \phi_\alpha \equiv Y_\alpha, \alpha = 1, 2, \ldots, N_s \), and \( \phi_{N_s+1} \) is the enthalpy. For a Newtonian fluid, with Fick’s law of diffusion, the viscous stress tensor \( \tau_{ij} \) and the scalar flux \( J_j^\alpha \) are represented by

\[
\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right), \quad J_j^\alpha = -\frac{\partial \phi_\alpha}{\partial x_j} \gamma,
\]

where \( \mu \) is the fluid dynamic viscosity, \( \gamma = \mu / Sc \) denotes the thermal and mass molecular diffusivity coefficients for all the scalars and \( Sc \) is the Schmidt number. Large eddy simulation involves the spatial filtering operation\(^{41,42}\)

\[
\langle Q(x,t) \rangle_\ell = \int_{-\infty}^{+\infty} Q(x',t)G(x',x)dx',
\]

where \( G(x',x) \equiv G(x' - x) \) denotes a filter function, and \( \langle Q(x,t) \rangle_\ell \) is the filtered value of the transport variable \( Q(x,t) \). In variable-density flows it is convenient to use the Favré-filtered quantity \( \langle Q(x,t) \rangle_L = \langle \rho Q \rangle_\ell / \langle \rho \rangle_\ell \). We consider a filter function that is spatially varying with the properties \( G(x) \geq 0 \) and \( \int_{-\infty}^{+\infty} G(x)dx = 1 \). Applying the filtering operation to Eq. (2.1) yields:

\[
\frac{\partial \langle \rho \rangle_\ell}{\partial t} + \frac{\partial \langle \rho \rangle_\ell \langle u_j \rangle_L}{\partial x_j} = 0
\]

\[
\frac{\partial \langle \rho \rangle_\ell \langle u_j \rangle_L}{\partial t} + \frac{\partial \langle \rho \rangle_\ell \langle u_i \rangle_L}{\partial x_j} = -\frac{\partial \langle p \rangle_\ell}{\partial x_i} + \frac{\partial \langle \tau_{ij} \rangle_\ell}{\partial x_j} + \frac{\partial \langle \phi_\alpha \rangle_\ell}{\partial x_j} \frac{\partial \tau_{ij}}{\partial x_j}
\]

\[
\frac{\partial \langle \rho \rangle_\ell \langle \phi_\alpha \rangle_L}{\partial t} + \frac{\partial \langle \rho \rangle_\ell \langle u_j \rangle_L \langle \phi_\alpha \rangle_L}{\partial x_j} = \frac{\partial \langle \gamma \frac{\partial \phi_\alpha}{\partial x_j} \rangle_\ell}{\partial x_j} - \frac{\partial M_j^\alpha}{\partial x_j} + \langle \rho S_\alpha \rangle_\ell
\]
where \( \Sigma_{ij} = \langle \rho \rangle L (\langle u_i u_j \rangle_L - \langle u_i \rangle_L \langle u_j \rangle_L) \) and \( M_j^a = \langle \rho \rangle L (\langle u_j \phi_a \rangle_L - \langle u_j \rangle_L \langle \phi_a \rangle_L) \) denote the SGS stress and the subgrid mass flux respectively. The filtered reaction source terms are \( \langle \rho S_\alpha \rangle_L = \langle \rho \rangle L (\langle S_\alpha \rangle_L - \langle u_j \rangle_L \langle \phi_a \rangle_L) \) and \( M_j^a = \langle \rho \rangle L (\langle S_\alpha \rangle_L - \langle u_j \rangle_L \langle \phi_a \rangle_L) \). In LES of non-reacting flows, the closure problem is associated with the subgrid stress term \( \Sigma_{ij} \) and the subgrid mass flux term \( M_j^a \). In reacting flows, an additional model is required for the filtered reaction rate, \( \langle \rho S_\alpha \rangle_L \). The latter modeling is the subject of FDF formulation described below. For the former two, we employ the standard Smagorinsky model applicable for a variable density flow:

\[
\Sigma_{ij} - \frac{2}{3} \langle \rho \rangle L C_\nu \Delta^2 S^2 \delta_{ij} = -2 \mu_t \left( \langle S_{ij} \rangle_L - \frac{1}{3} \langle S_{kk} \rangle_L \delta_{ij} \right), \quad M_j^a = -\gamma_t \frac{\partial \langle \phi_a \rangle_L}{\partial x_j} \tag{2.7}
\]

The filtered strain rate tensor \( \langle S_{ij} \rangle_L \) is given by:

\[
\langle S_{ij} \rangle_L = \frac{1}{2} \left[ \frac{\partial \langle u_i \rangle_L}{\partial x_j} + \frac{\partial \langle u_j \rangle_L}{\partial x_i} \right] \tag{2.8}
\]

The eddy-viscosity is modeled by \( \mu_t = \langle \rho \rangle L [C_{\nu_1} \Delta]^2 S \), where \( C_{\nu_1} = 0.2, \ C_{\nu_2} = 0.18, \ \gamma_t = \mu_t / Sc_t \), \( Sc_t = 1 \), \( S = \sqrt{2 \langle S_{ij} \rangle_L \langle S_{ij} \rangle_L} \). The parameter \( \Delta \) denotes the characteristic filter size and is taken as \( \Delta = [V_{cell}]^{1/3} \), where \( V_{cell} \) denotes the cell volume. It must be pointed out that commutation of filtering and differentiating operations is a prerequisite for the derivation of the filtered equations. The commutation error in the unstructured mesh formulation is ignored here. The complete SGS statistical information of the scalars is contained within the scalar filtered mass density function (SFMDF). This is defined as:

\[
F_L (\psi, x, t) = \int_{-\infty}^{+\infty} \rho(x', t) \zeta (\psi, \phi(x', t)) G(x' - x) dx', \tag{2.9}
\]

where

\[
\zeta (\psi, \phi(x, t)) = \prod_{\alpha=1}^{\sigma} \delta (\psi_\alpha - \phi_\alpha(x, t)). \tag{2.10}
\]

In this equation, \( \delta \) denotes the Dirac delta function, and \( \psi \) represents the scalar array in the sample space. The term \( \zeta \) is the “fine-grained” density. Equation (2.9) defines SFMDF as the spatially filtered value of the fine-grained density. With the condition of a positive filter
kernel,48 $F_L$ has all the properties of a mass density function.47 Defining the “conditional filtered value” of $Q(x, t)$ as

$$\langle Q \mid \psi \rangle_\ell \equiv \frac{\int_{-\infty}^{+\infty} Q(x', t) \rho(x', t) G(x' - x) \, dx'}{F_L(\psi, x, t)},$$

(2.11)

the SFMDF is governed by the exact transport equation5

$$\frac{\partial F_L}{\partial t} + \frac{\partial[\langle u_j(x, t) \mid \psi \rangle_\ell F_L]}{\partial x_j} = -\frac{\partial}{\partial \psi_\alpha} [S_\alpha(\psi) F_L] + \frac{\partial}{\partial \psi_\alpha} \left[ \langle \frac{1}{\rho(\phi)} \frac{\partial J_\beta^\alpha}{\partial x_j} \mid \psi \rangle_\ell F_L \right].$$

(2.12)

This equation indicates that the effect of chemical reaction (the first term on RHS) appears in a closed form. The unclosed nature of SGS convection and mixing is indicated by the conditional filtered values in the other two terms. To close these terms, we use a gradient diffusion model for convection, and the linear mean square estimation (LMSE) model10,11 for molecular mixing. These are given in terms of the stochastic differential equations (SDE’s):41,46

$$dX^+_i(t) = \left[ \langle u_i \rangle_L + \frac{1}{\langle \rho \rangle_\ell} \frac{\partial (\gamma + \gamma_i)}{\partial x_i} \right] dt + \sqrt{2(\gamma + \gamma_i)/\langle \rho \rangle_\ell} dW_i(t),$$

(2.13)

$$d\phi^+_\alpha = -\Omega_m (\phi^+_\alpha - \langle \phi_\alpha \rangle_L) \, dt + S_\alpha(\phi^+) \, dt.$$  

(2.14)

where $dW_i$ is the Weiner-Levy process49 and, $X^+_i$ and $\phi^+_\alpha$ are probabilistic representations of the position and the scalar variables, respectively. In the model, $\Omega_m = C_\phi (\gamma + \gamma_i) / (\langle \rho \rangle_\ell \Delta^2)$ is the SGS mixing frequency and $C_\phi = 4$ is a model constant. The Fokker-Planck equation corresponding to this model is:50

$$\frac{\partial F_L}{\partial t} + \frac{\partial[\langle u_j \rangle_L F_L]}{\partial x_j} = \frac{\partial}{\partial x_j} \left[ (\gamma + \gamma_i) \frac{\partial (F_L/\langle \rho \rangle_\ell)}{\partial x_j} \right] + \frac{\partial}{\partial \psi_\alpha} \left[ \Omega_m(\psi_\alpha - \langle \phi_\alpha \rangle_L)F_L \right] - \frac{\partial[S_\alpha F_L]}{\partial \psi_\alpha}.$$  

(2.15)

Equation (2.15) represents the modeled FDF transport equation.
2.2 FDF ON UNSTRUCTURED GRIDS

The extent of previous contributions in PDF simulations on unstructured mesh is somewhat limited;\textsuperscript{51–54} for FDF it is nonexistent! To facilitate FDF-LES on unstructured grids, here a Lagrangian Monte Carlo (MC) methodology is developed and is overlayed on a domain portrayed by an unstructured mesh. Details of the MC solver for FDF are described in several previous works; see Ref.\textsuperscript{55} for a tutorial. Here, the basic elements of the simulations on unstructured grids are described.

The FDF is represented by an ensemble of $N_p$ stochastic particles, each carrying information pertaining to it’s position, $X^n(t)$ and scalar values, $\phi^n(t)$, $n = 1, 2, ..., N_p$. This information is updated by the temporal integration of the SDE’s (Eqs. (2.13)-(2.14)). The computational domain is discretized into unequally spaced tetrahedral cells. These cells are used for two purposes: (1) to identify the regions where the statistical information from the MC simulations are obtained; (2) to perform LES via the FV coupled to the MC solver. The LES procedure via the FV discretization is referred to as LES-FV. The MC particles require the input of the filtered mean velocity and the diffusivity (molecular and subgrid). These are provided by the LES-FV solver on the fixed grids and are interpolated to the particle location. The LES of hydrodynamic variables is conducted on the unstructured mesh using a segregated, collocated and implicit pressure-based algorithm. A second order accurate bounded central discretization scheme is employed for solution of the filtered equations. The bounded central difference scheme is a composite normalized variable diagram (NVD) scheme\textsuperscript{56} and consists of a blended scheme of central differencing and a second order upwind scheme. For the temporal term, a fully implicit, second order accurate backward discretization scheme is used. For the MC solution, a splitting procedure is employed in which mixing and reaction in the composition domain are treated separately. In the latter:

$$\phi(t) \rightarrow^{\text{mixing}} \langle \phi \rangle(t) + [\phi(t) - \langle \phi \rangle(t)] e^{-\Omega_m \Delta t} \rightarrow^{\text{reaction}} \phi(t + \Delta t) \quad (2.16)$$

The statistics are evaluated by consideration of particles within a volume centered at the point of interest. Effectively, this volume constitutes an “ensemble domain” characterized by the length scale $\Delta_E$ in which the FDF is discretely represented. This is illustrated in Fig.
showing tetrahedral and spherical ensemble domains. For reliable statistics with minimal dispersion, it is required to maximize the number of particles and to minimize the size of the ensemble domain. To maximize accuracy with finite number of particles, a variant of the “basis function method” for mean estimation is implemented. To describe this variant, consider a generic cell element $E$ having $N^E_v$ vertices. Point $P$ denotes the location of the MC particle $j$ within this cell. A basis function for a vertex $i (i = 1, 2, ..., N^E_v)$ of the cell $E$ with respect to the particle $j$ is given by:

$$b^E_{ij} = \frac{1}{1 + r_{ij} \sum_{k=1, k \neq i}^{N^E_v} \frac{1}{r_{kj}}}$$

(2.17)

where $r_{ij}$ is the distance between the vertex $i$ and the particle $j$. Let $C_i$ be the number of cells sharing the vertex $i$. An estimate of the mean scalar values at the vertex $i$ can be obtained by summing over all the particles in the cells which share the vertex and taking into account the vertex basis functions:

$$\langle \phi_i \rangle_L = \sum_{E \subset C_i} \sum_{j=1}^{N^E_p} m_j b^E_{ij} \phi_j$$

(2.18)

where $N^E_p$ denotes the number of particles in cell $E$ and $m_j$ is the mass of the particle $j$. Within the cell, the scalar mean values at the particle location $j$ can be expressed in terms of the vertex mean values as estimated above and the basis functions:

$$\langle \phi^E_j \rangle_L = \sum_{i=1}^{N^E_v} b^E_{ij} \langle \phi_i \rangle_L$$

(2.19)

An error estimate of the basis function method is provided by considering the canonical problem of fitting a random particle data $\Xi(X_i, Y_i)$ to a function $m(X_i, Y_i)$. This function is chosen as:

$$m(X_i, Y_i) = 3X_i^2Y_i^2 \sin(\pi X_i) \sin(\pi Y_i)$$

(2.20)
within a square domain (of size $1 \times 1$) covered by unstructured grids. The random particle data $\Xi(X_i, Y_i)$ is modeled as

$$\Xi(X_i, Y_i) = m(X_i, Y_i) + \sigma \xi_i$$

(2.21)

where $\xi_i$ is a random variable with standard Gaussian PDF and $\sigma$ is a measure of the noise in the particle data. Figure 2 shows contour plots of the function $m(X_i, Y_i)$, and the noisy particle field $\Xi(X_i, Y_i)$ for $\sigma = 0.05$. The error $\epsilon(X_i, Y_i)$ is obtained by constructing an estimate $\hat{\Xi}(X_i, Y_i)$ for the function $m(X_i, Y_i)$ and evaluating:

$$\epsilon(X_i, Y_i) = \Xi(X_i, Y_i) - m(X_i, Y_i).$$

(2.22)

The total RMS error $\epsilon_t$ is comprised of the discretization error, the bias error, and the statistical error. This error is monitored as a function of the average grid size $\Delta_{avg}$, the noise $\sigma$, and the number of particles $N_{pE}$ within each cell.

$$\epsilon_t = \sqrt{\frac{1}{N} \sum_{i=1}^{N} [\hat{\Xi}(X_i, Y_i) - m(X_i, Y_i)]^2}$$

(2.23)

where $N = \sum N_{pE}$ is the total number of particles within the entire domain. Seven mesh configurations with a total mesh count in the range $100-5000$, and five noise levels $\sigma \approx 0.05-0.3$ are considered. Figure 3(a) shows the variations of $m(X_i, Y_i)$ and $\Xi(X_i, Y_i)$ at $Y = 0.75$ as a function of the average grid size. The number of particles per cell is kept fixed at 40 with $\sigma = 0.1$. This figure provides a visual measure of the discretization error. As expected, the difference between $m(X_i, Y_i)$ and $\Xi(X_i, Y_i)$ is the maximum for the coarsest mesh. In Fig. 3(b) the noise level is varied by keeping the average grid size fixed, $\Delta_{avg} = 0.037992$ (corresponding to a mesh count of 1600), with 40 particles per cell. It is shown that an increase in noise causes an increase in the estimated error. Finally, Fig. 4 gives the total RMS error as a function of the average grid size $\Delta_{avg}$. As expected, the total error decreases as the mesh size decreases with the approximate scaling of $\Delta_{avg}^2$.

Solution of the stochastic differential equation (2.13) requires the input of the filtered velocity, the diffusion coefficient and gradients of the scalars field at the particle locations. These are provided by the FV solution and subsequent interpolation to the particle locations.
Figure 5 provides a schematic of a tetrahedral cell showing its center $C$, and containing the MC particles. A typical particle is located at $P$, a distance of $\vec{r}$ from the center. $\vec{A}_F$ is the normal vector on a face of the cell. The interpolation at the particle location is done via a second order piecewise linear reconstruction method:

$$\phi_P = \phi_C + \zeta_C (\nabla \phi_C \cdot \vec{r})$$  \hspace{1cm} (2.24)

where $\phi_P$ and $\phi_C$ denote the values at the particle location and the cell center, respectively. The parameter $\zeta_C$ denotes a limiter function\textsuperscript{57} which prohibits the linearly reconstructed field variable at the particle location to exceed the maximum or minimum values of the neighboring cells. $\nabla \phi_C$ is evaluated at the cell center via the Green-Gauss theorem. For efficient tracking of the MC particles including their mesh compartment, a new procedure is developed here which is effective for unstructured mesh simulations. The essence of this procedure is described via Fig. 6 (in 2D for clarity). A particle is located within cell $i$ at location $P_A$ at time $t$. A cell pointer identifies the particle with its cell host. The particle undergoes a displacement as per the stochastic model given by Eq. (2.13) over a time-step $\Delta t$. $P_B$ and $P_C$ are two possible positions of the particle at time $t + \Delta t$. $P_B$ represents a position which is inside the original cell and $P_C$ represents a position in one of the neighboring cells $j$. The time-step is chosen so that at least one step is taken by the particle in the cell in which it is traversing. After a time-step, the location of the particle is monitored to determine whether it has left the cell or not. This is done by computing the normal distance of the particle from the faces of the cell:

$$h_{i1,2,3}^{1,2,3} = (\vec{r}_F - \vec{r}_P) \bullet \vec{n}_{i1,2,3}^{1,2,3}$$  \hspace{1cm} (2.25)

where $h_{i1,2,3}^{1,2,3}$ is the particle to face normal distance for cell $i$ for the three faces $(1, 2, 3)$. The parameters $\vec{r}_F$ and $\vec{r}_P$ are the position vectors of the centroid of the face $F$ and the particle $P$ respectively from the global origin; and $\vec{n}_{i1,2,3}^{1,2,3}$ is the outward unit normal on the face of the cell $i$. The particle is in cell $i$ at location $P_B$ if all the particle to face normal distances $h_{i1,2,3}^{1,2,3}$ are positive. If not, the neighboring cells are searched to locate the particle. If it is found in cell $j$, the cell pointer of the particle is updated from $i$ to $j$. 

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2.3 DEMONSTRATION

In this section, results are presented of the FDF solver on unstructured grids for LES of a three-dimensional, temporally developing mixing layer. This layer consists of two parallel streams traveling in opposite directions with the same speed. In the representation below, \( x, y \) and \( z \) denote the stream-wise, the cross-stream and the span-wise flow directions respectively (Fig. 7). The velocity components in these directions are denoted by \( u, v \) and \( w \). The filtered stream-wise velocity is initialized with a hyperbolic tangent profile with \( \langle u \rangle_L = 1 \) on the top stream and \( \langle u \rangle_L = -1 \) on the bottom stream. The simulations are conducted on a cube box, \( 0 \leq x \leq L, -L/2 \leq y \leq L/2 \) and \( 0 \leq z \leq L \). The box length \( L \) is specified such that \( L = 2^{n_p} \lambda_u \), where \( n_p \) is the desired number of successive vortex pairings and \( \lambda_u \) is the wavelength of the most unstable mode corresponding to the mean stream-wise velocity profile imposed at the initial time. The flow variables are normalized with respect to the half initial vorticity thickness, \( L_r = [\delta_v (t = 0)/2] ; \delta_v = \Delta U / |\partial \langle u \rangle / \partial y|_{\text{max}} \), where \( \langle u \rangle \) is the Reynolds averaged value of the filtered stream-wise velocity and \( \Delta U \) is the velocity difference across the layer. The reference velocity is \( U_r = \Delta U / 2 \). The Reynolds number based on the reference velocity and length scales is \( Re = 50 \). The formation of the large scale vortical structures are expedited through eigenfunction based initial perturbations. This includes 2D and 3D perturbations with a random phase shift between the 3D modes. This results in the formation of two successive vortex pairings and strong three dimensionality.

Both non-reacting and reacting layers are considered. In the non-reacting flow, trace of a passive scalar \( \phi \) is considered. This is again initialized as a hyperbolic tangent profile with \( \langle \phi \rangle_L = 1 \) on the top stream and \( \langle \phi \rangle_L = 0 \) on the bottom stream. In the reacting case, an irreversible, second-order reaction scheme of type \( A + rB \rightarrow (1 + r)P \) is considered. The reactant conversion is governed by \( S_A = -k_r AB \), where \( k_r \) is the reaction rate constant; and \( A, B \) denote the mass fractions of the two reactants. The scalar field is initialized as \( A \equiv \phi \) (as described above) and \( B = 1 - A \). All of the species (\( A, B, P \)) are considered thermodynamically identical, and the fluid is assumed calorically perfect. The degree of exothermicity is parameterized by \( C_E = -\Delta h^0_p / (C_p T_r) \) where \( \Delta h^0_p \) is the heat of reaction, \( C_p \) is the specific heat at constant pressure, and \( T_r = 298.15K \) denotes the reference ambient
temperature. In the simulations below, $C_E = 0.086$ is kept fixed. The rate of reactant conversion is parameterized by the Damköhler number, $Da = k_r L_r / U_r$. Simulations are conducted with relatively slow ($Da = 10$) and fast ($Da = 10^6$) reaction rates.

Simulations are conducted on an unstructured tetrahedral mesh (Fig. 7) with a total mesh count of 294,273. The MC particles are initially distributed somewhat uniformly throughout the domain. The initial number of particles per cell is 60. Figure 7 shows the distribution of MC particles inside the cube with unstructured mesh at an intermediate time. The simulated results are analyzed both instantaneously and statistically. In the former, the snap-shot contours and scatter plots of the scalar variable are displayed. In the latter, the Reynolds averaged statistics are considered. These are constructed by spatial averaging over $x$ and $z$ directions. All Reynolds averaged results are denoted by an over-bar. First, we check the consistency of the simulator. This is best achieved by comparing the lower moments as obtained from FDF with those simulated directly via LES-FV on the same mesh. The chemical source terms are evaluated solely via the MC solver and are then used in the FV solution of the filtered species equations. Therefore the filtered scalar values are obtained via both FV and MC. This “redundancy” is very useful in establishing the consistency of the hybrid solver. Some of the FDF predictions are also compared against direct numerical simulation (DNS) data of Sheikhi et al.\textsuperscript{6,7}

In Fig. 8 results are presented of the instantaneous contour plots of the filtered scalar ($\phi$) field. This figure provides a visual demonstration of the consistency of the FDF simulator as the MC results are in agreement with those via LES-FV. This is corroborated quantitatively by the scatter plots of the instantaneous filtered values in Fig. 9 and the cross-stream variation of the Reynolds averaged statistics in Fig. 10. The latter also indicates that the magnitude of the filtered field is somewhat insensitive to the shape and the size of the ensemble domain. This is not the case for the SGS second-order moment $\tau(\phi, \phi)$, $\tau(a, b) = \langle ab \rangle_L - \langle a \rangle_L \langle b \rangle_L$ as shown in Fig. 11. This figure indicates that the FV and the MC solutions merge as the size of the ensemble domain is reduced. The best agreement is obtained with a spherical ensemble domain with $\Delta_E = \Delta / 2$. The resolved components of the Reynolds averaged variance $R(\phi, \phi)$, $R(a, b) = \left( \langle a \rangle_L - \langle a \rangle_L \right) \left( \langle b \rangle_L - \langle b \rangle_L \right)$ are also consistently calculated with the two solvers as shown in Fig. 12. Hereinafter, unless other-
wise noted, statistics are generated with consideration of a spherical ensemble domain with $\Delta_E = \Delta/2$.

To assess the effects of grid resolution, simulations are conducted on four mesh configurations (G1 to G4) with a progressively increasing resolution. The coarsest mesh (G1) consists of 50,000 tetrahedral elements. Configurations G2 and G3 contain 100,000 and 200,000 elements, respectively; and the finest mesh G4 has 294,273 elements. Figure 13 shows the FDF predictions of the scalar mean values, the resolved variance, and the total variance, $\overline{r(\phi, \phi)}$, $r(a, b) = (a - \overline{a})(b - \overline{b})$. It is demonstrated that as the resolution increases, the FDF predictions become closer to the DNS results. The agreement is best for the G4 configuration. This level of agreement is the same as that previously observed via high order finite difference LES on structured equally spaced grids.\textsuperscript{6,7}

In the reacting case, the consistency of the FMDF calculations and realizability of the simulated results are investigated. The consistency is qualitatively established in Fig. 14 via the instantaneous contour plots of the filtered temperature field. This is corroborated quantitatively by the corresponding scatter plots and the Reynolds-averaged values as shown in Figs. 15 and 16, respectively. To assess realizability, the temperature and scalar values of the MC particles in the domain of the “mixture fraction” $F$\textsuperscript{58} are shown in Figs. 17 and 18. For the case with moderate chemistry $Da = 10$, the compositional structure is similar to that of a distributed reaction zone.\textsuperscript{59} For the case with fast chemistry, $Da = 10^6$, the structure is similar to that of a thin flame sheet.\textsuperscript{60} For further assessment of realizability, the behavior of two Shvab-Zeldovich (conserved scalar) variables\textsuperscript{61} are considered:

$$Z2 = \frac{A - \frac{B}{r} + \frac{B_a}{r}}{A_0 + \frac{B_a}{r}} \quad Z3 = \frac{A + \frac{C_p}{\Delta h_p(r+1)}(T - T_B)}{A_0 + \frac{C_p}{\Delta h_p(r+1)}(T_A - T_B)}$$ \hspace{1cm} (2.26)

where the subscript 0 denotes the free stream values; and $T_A$, $T_B$ refer to the temperatures in the top and bottom streams, respectively. Figures 19 and 20 show the scatter plots of these variables against each other, and against another conserved scalar transport variable $Z1$ calculated directly from LES-FV in a constant density, non-reacting flow simulation. As shown, the correlation between $Z2$ an $Z3$ is excellent; but not between either of these two and $Z1$. This is primarily due to the variation of density in the reacting flow simulations.
The correlation between the product formation and the rise in temperature is also excellent as shown by the scatter plots of \((-\Delta h_0^p P/C_p)\) vs. the temperature rise \((T - T_r)\).

\[2.4\] CHAPTER SUMMARY

The filtered density function (FDF) has proven to be a viable tool for large eddy simulation (LES) of turbulent combustion. In all of the previous contributions, the FDF is simulated on structured grids. The primary objective of the present work is to provide a FDF simulator on unstructured meshes. This simulator is based on a Lagrangian Monte Carlo (MC) FDF solver which is constructed on a domain portrayed by an unstructured mesh. The base filtered flow equations on this mesh are solved via a finite-volume (FV) method. The MC and the FV solvers are tightly coupled. The MC particle properties evolve according to modeled stochastic differential equations (SDEs). These SDEs require the input of the filtered velocity, its gradient and the diffusion coefficients. These are computed via the FV solver. The filtered value of the chemical reaction conversion rate is obtained via the MC solver. Thus, the filtered scalar fields are determined via both FV and MC. This redundancy provides a convenient means of establishing consistency. An efficient methodology is developed to track particles in the setting of the unstructured mesh and to interpolate the cell variables to the particle location. In addition, several sampling domains are considered for evaluation of the filtered values from the MC solver. The overall capability of the unstructured FDF simulator is assessed via LES of a temporally developing turbulent mixing layer under both non-reacting and chemically reacting conditions. The consistency and realizability of the simulated results are established and the predictive capability of FDF is demonstrated via comparison with direct numerical simulation (DNS) data.
Figure 1: Ensemble averaging on unstructured mesh. 1: tetrahedral with $\Delta_E = \Delta$, 2: spherical with $\Delta_E = \Delta$, 3: spherical with $\Delta_E = \Delta/2$. Solid circles denote the MC particles and the open circle denotes the centroid of the triangular cell. Diagram not to scale.
Figure 2: (a) Contour plot of function $m(X_i, Y_i)$, (b) contour plot of function $\Xi(X_i, Y_i)$ with noise $\sigma = 0.05$. 
Figure 3: Functions $m(X_i, Y_i)$ and $\hat{\Xi}(X_i, Y_i)$ at $y = 0.75$. (a) $N^E_p = 40$ and $\sigma = 0.1$, (b) $\Delta_{avg} = 0.037992$ and $N^E_p = 40$. 
Figure 4: RMS error $\epsilon_t$ vs. average grid size $\Delta_{avg}$ for $N_p^E = 40$. 

\[
\sigma = 0.05 \\
\sigma = 0.1 \\
\sigma = 0.15 \\
\sigma = 0.2 \\
\sigma = 0.3 \\
\]
Figure 5: Random distribution of MC particles within a tetrahedral cell. The open circle denotes the cell centroid and the solid circles denote the MC particles. The solid squares denote the cell vertices.
Figure 6: Particle movement in an unstructured mesh. The open circles denote the cell centroids, the solid circles denote the particle locations and the solid squares denote the cell vertices.
Figure 7: Unstructured tetrahedral mesh for the temporal mixing layer and the distribution of Monte-Carlo particles within the domain at an intermediate time. The particles are colored by their scalar values.
Figure 8: Contour plots of the filtered scalar field at $t = 80$. (a) FV, (b) MC.
Figure 9: Scatter plot of the filtered values of the scalar as obtained by SFDF vs. those obtained by LES-FV at $t = 80$. The correlation coefficient is 0.9988.
Figure 10: Cross-stream variation of the Reynolds-averaged values of the filtered scalar field at two different times. The thick solid line denotes LES-FV prediction and the remaining symbols denote SFDF predictions. * = Basis function method; + = Tetrahedral ensemble of size $\Delta_E = \Delta$; x = Spherical ensemble of size $\Delta_E = \Delta$; o = Spherical ensemble of size $\Delta_E = \Delta/2$. (a) $t = 60$, (b) $t = 80$. 

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Figure 11: Cross-stream variation of the Reynolds averaged SGS scalar variance. The solid circles denote LES-FV results and the other lines denote FDF predictions. (a) $t = 60$, (b) $t = 80$. 
Figure 12: Cross-stream variation of the Reynolds-averaged values of the resolved scalar variance. The thick solid line denotes FDF predictions and the solid circles denotes LES-FV data. (a) $t = 60$, (b) $t = 80$. 
Figure 13: Cross-stream variation of the Reynolds averaged (a) scalar mean, (b) resolved variance and (c) total variance at $t = 60$ for various grid configurations.
Figure 14: Contour plots of the temperature field (in Kelvin units). (a) FDF, (b) LES-FV.
Figure 15: Scatter plot of the filtered temperature field (in Kelvin units) as obtained by MC vs. those via LES-FV. The correlation coefficient is 0.9984.
Figure 16: Cross-stream variation of the Reynolds averaged filtered temperature field (in Kelvin units). The thick solid line denotes MC results and the solid circles denote LES-FV predictions.
Figure 17: Scatter plots of filtered temperature $\langle T \rangle_L$ vs. the filtered mixture fraction $\langle F \rangle_L$ between the pure mixing and the infinitely fast chemistry bounds. (a) $Da = 10$, (b) $Da = 10^6$. 
Figure 18: Scatter plots of filtered species mass fraction $\langle A \rangle_L$ vs. the filtered mixture fraction $\langle F \rangle_L$ between the pure mixing and the infinitely fast chemistry bounds. (a) $Da = 10$, (b) $Da = 10^6$. 
Figure 19: (a) Scatter plot of the filtered $\langle Z1 \rangle_L$ vs. the filtered $\langle Z2 \rangle_L$ as obtained by the MC solution. The correlation coefficient is 0.9987. (b) Scatter plot of the filtered $\langle Z1 \rangle_L$ vs. the filtered $\langle Z3 \rangle_L$ as obtained by the MC solution. The correlation coefficient is 0.9987.
Figure 20: (a) Scatter plot of the filtered $\langle Z_2 \rangle_L$ vs. the filtered $\langle Z_3 \rangle_L$ as obtained by MC solution. (b) Scatter plot of the filtered $\langle -\Delta h^0_p P/C_p \rangle_L$ vs. the filtered $\langle T - T_r \rangle_L$ as obtained by the MC solution.
3.0 FDF SIMULATION OF SWIRLING REACTING FLOWS

In the work described in this chapter, the unstructured S-FMDF methodology as discussed in Chapter 2, is employed for large eddy simulation of two swirl stabilized non-premixed flames. These are low-swirl (SM1) and high-swirl (SMA2) methane flames; both of which have been the subject of detailed laboratory measurements.\(^1\) Combustion chemistry is modeled via a flamelet model for SM1, and a detailed finite rate kinetics model\(^62\) for SMA2. The S-FMDF is simulated by a Lagrangian Monte Carlo method. The simulated results are assessed via comparison with experimental data and show excellent agreements. The grid dependency of the predicted results for (SM1) is also assessed via consideration of a progressively increasing mesh resolution. The assessment indicates that the results converge to the measured data as the grid resolution increases. This demonstrates the capability of S-FMDF for LES of complex flows, and warrants future applications of the methodology for LES of practical combustor configurations.

3.1 FLAME CONFIGURATIONS

The schematic of the Sydney swirl burner\(^1\) as considered in our simulations is shown in Fig. 21. The burner has a 50 \(mm\) diameter bluff body with a 3.6 \(mm\) central fuel jet. The bluff-body is surrounded by a 60 \(mm\) diameter annulus for the primary swirling air stream. The combustor is situated in a tunnel providing a co-flowing, secondary air stream of 20 \(m/s\) with a free-stream turbulence level of 2 percent. The flame structure is varied by changing the bulk flow, and swirl velocities. In the experiments,\(^1\) eight turbulent flames are considered. The geometrical configuration in these flames is the same, but the inlet jet
composition and swirl numbers are varied. Two of these flames are targeted for our model validations: SM1 and SMA2. In SM1, the central fuel stream is pure methane and has a bulk velocity of 32.7 m/s. The swirling air stream has an axial bulk velocity of 38.2 m/s and a bulk tangential velocity of 19.1 m/s. In SMA2, the central jet is 1 : 2 CH₄-air with a bulk velocity of 66.3 m/s and the swirling air stream has an axial velocity of 16.3 m/s and a bulk tangential velocity of 25.9 m/s.

The SM1 flame is simulated using the flamelet model. The model is constructed by considering the one-dimensional counterflow laminar flame in which the chemical reaction is described via detailed chemical kinetics. At low strain rates, all the thermo-chemical variables are considered a function of the mixture fraction (Z) only. The detailed kinetics mechanism of the Gas Research Institute (GRI 2.11) is employed to describe combustion, and the flamelet table at a strain rate of $a = 300 \text{ 1/s}$ is used to relate the thermo-chemical variables to the mixture fraction. For this fixed value of $a$, the SGS statistics of the thermo-chemical variables are determined from the S-FMDF:

$$
\langle \phi(\mathbf{x},t) \rangle_L = \frac{1}{\langle \rho \rangle_L} \int \phi(\xi)F_L(\xi, \mathbf{x}, t) d\xi.
$$

(3.1)

where $\xi$ denotes the probability space of the mixture fraction. The SMA2 flame is simulated using a 46-step 17-species finite rate chemistry mechanism of Smooke et al. The ISAT algorithm is employed for the chemical kinetics calculations.

3.2 RESULTS

The LES domain starts from the exit of the burner assembly; see Fig. 21. An ensemble of tetrahedrons covers the entire cylindrical combustor that spans an axial length of 350 mm and a diameter of 100 mm in the radial direction. The parts containing the central fuel stream and the primary swirling air stream are modeled via Reynolds-averaged Navier Stokes (RANS). Random perturbations somewhat similar to that in Ref. are added to this mean field to generate “turbulent fluctuations” for the LES region.
To assess the grid resolution dependency of the FDF simulation in SM1 flame, three mesh configurations (G1 to G3) with a progressively increasing number of elements are considered. The coarsest mesh (G1) has a total cell count of 940,000 elements and the finest mesh (G3) has a count of 2,140,000 mesh elements. Configuration G2 in between has a cell count of 1,400,000 elements. The FMDF solver is initialized with 30 particles per cell. The particles are supplied at the inlet and move within the domain due to the combined actions of convection and diffusion (molecular and SGS). During the course of SM1 simulations, the total number of particles in the domain are in the range of 29 – 65 million. The mesh count in SMA2 flame is 1,850,000 tetrahedral elements. The FMDF solver in SMA2 is also initialized with 30 MC particles per cell. 60 million particles are tracked during the course of SMA2 simulation. The simulations are conducted for 8 flow-through times (based on the jet bulk axial velocity). The results are monitored to ensure that the particles fully encompass and extend well beyond regions of non-zero vorticity and reaction. The Reynolds-averaged statistics, to be compared with experimental data, are obtained by a long time (5 flow-through time) averaging of the filtered field. A total of 16,000 samples are collected in this recording period. The notations $\bar{Q}$ and $RMS(Q)$ denote respectively, the Reynolds-averaged mean and root mean square values of the variable $Q$. For the RMS, the contributions of both the resolved and the subgrid counterparts are included. The results are not averaged over the azimuthal directions.

Figures 22(a) and (b) show the instantaneous flow and flame structures in SM1 and SMA2 respectively. The flow pattern in SM1 shows a complex structure with a toroidal recirculation zone at the base of the bluff body. Downstream of the first recirculation zone, the flame shows a “neck” region where intense turbulence-chemistry interactions are observed. A second recirculation zone appears further downstream of the neck region. A steady stream of vortices are shed by both the fuel and primary air streams. They intermix as they travel downstream. The SMA2 flame shows a single recirculation zone near the bluff body. No necking phenomenon or vortex shedding is observed. This is partly due to the higher axial fuel velocity in SMA2. Figure 23 shows the toroidal flow structure for SM1 visualized by iso-surface of the second invariant of the velocity deformation tensor colored by velocity and Fig. 24 shows the swirl structure exhibited by a fraction of fluid particles in SM1. The particles
are colored by temperature. To assess consistency, Fig. 25 shows the instantaneous density field as obtained via both MC and FV for SM1 flame. The latter shows some numerical diffusion which is absent in the Lagrangian simulations.

The capability of the model in predicting the hydrodynamic field is demonstrated by examining some of the radial distributions of the flow statistics in SM1 at several axial locations (Fig. 26). The peak value of the mean axial and swirl velocity profiles and the spread of the jet is predicted well by all the mesh configurations but the results for G3 compares best with experimental data. Figure 27 shows that the mean values of the mixture fraction, the RMS of the mixture fraction and the mean temperature are also predicted quite well. Again, the values converge to the experimental data with mesh refinement. The statistics of the mass fractions of several of the species (CO, OH, H₂O, CO₂) at different stream-wise locations are compared with measured data in Fig. 28. The mean profiles of the species show close agreement with measurements. The discrepancy observed at some locations is attributed in part to the use of a single flamelet table. The use of multiple flamelet tables might be able to address this discrepancy.

The Reynolds averaged axial and swirl velocity profiles at several locations for SMA2 flame are shown in Fig. 29. The peak location and the magnitudes are predicted reasonably well. Figure 30 indicates that the mean values of the mixture fraction, the rms of the mixture fraction and the mean temperature for SMA2 are all predicted well by the model. Finally the statistics of the mass fractions of several of the species (CO, OH, H₂O, CO₂) at different stream-wise locations are compared with measured data in Fig. 31. The overall agreement with experiments is very good except for the minor species OH. It is anticipated that the discrepancy observed in SMA2 OH results may be eliminated if a more detailed kinetics model is used. The asymmetry of some of the results, as also observed experimentally, would be reduced by increasing the number of realizations in acquiring the statistics.
3.3 CHAPTER SUMMARY

Since its original development a decade ago, FDF has experienced widespread application for LES of a variety of turbulent reacting flows.\textsuperscript{40} The present work demonstrates that FDF can now be considered for LES of complex flames. This is done by implementation of the scalar filtered mass density function (S-FMDF) on a domain portrayed by an unstructured grid. The modeled transport equation for S-FMDF is solved by a Lagrangian Monte Carlo method, coupled with the finite-volume solution of the transport flow variables. The resulting FV/MC solver is employed for LES of two swirl-stabilized flames as considered in Sydney experiments:\textsuperscript{1} a low-swirl (SM1), and a high-swirl (SMA2) one. Combustion chemistry is modeled via a flamelet model for SM1, and a detailed finite rate kinetics model\textsuperscript{62} for SMA2. The predictive capability of the model is assessed by comparison of the Reynolds-averaged statistics of the thermo-chemical variables with measured data. In general, excellent agreements are observed. The grid dependency of the predicted results is also assessed via consideration of a progressively increasing mesh resolution for SM1. In the case with the finest mesh resolution, there are over 2 million mesh elements within the domain. The results of this resolution assessment indicate that all of the moments converge to the measured data as the grid resolution increases. The best agreement is observed for the case with the highest number of elements as most of the thermo-chemical variables are correctly predicted.
Figure 21: Schematic of flow configuration with tetrahedral mesh elements. Flow direction is from right to left.
Figure 22: Flame structure depicted by the instantaneous flow vectors colored by the filtered temperature values (a) SM1, (b) SMA2. Flow direction is from right to left.
Figure 23: Flow structure for SM1 visualized by iso-surface of the second invariant of the instantaneous velocity deformation tensor colored by filtered velocity. Flow direction is from right to left.
Figure 24: Distribution of a fraction of fluid particles depicting swirl in SM1. The particles are colored by the filtered temperature values. Flow direction is from right to left.
Figure 25: Density field in the central $r - Z$ plane in SM1 via (a) MC and (b) FV. Flow direction is from bottom to top.
Figure 26: Radial distribution of Reynolds averaged axial velocity $\langle U \rangle_L$ and swirl velocity $\langle W \rangle_L$ in SM1 at $z = 20$ mm (left) and $z = 70$ mm (right). G1: thin line, G2: dashed line, G3: bold line, Circles: experiment.¹
Figure 27: Radial distribution of Reynolds averaged mixture fraction $\langle Z \rangle_L$, total $\text{RMS}(Z)$ and temperature $\langle T \rangle_L$ in SM1 at $z = 20$ mm (left) and $z = 75$ mm (right). G1: thin line, G2: dashed line, G3: bold line, Circles: experiment.\textsuperscript{1}
Figure 28: Radial distribution of Reynolds averaged $\langle Y_{CO} \rangle_L$, $\langle Y_{OH} \rangle_L$, $\langle Y_{H_2O} \rangle_L$ and $\langle Y_{CO_2} \rangle_L$ in SM1 at $z = 20$ mm (left) and $z = 75$ mm (right). G1: thin line, G2: dashed line, G3: bold line, Circles: experiment.¹
Figure 29: Radial distribution of Reynolds averaged axial velocity $\langle U \rangle_L$ and swirl velocity $\langle W \rangle_L$ in SMA2 at $z = 20$ mm (left), $z = 50$ mm (middle) and $z = 100$ mm (right). The thick solid line denotes SMFDF predictions and the circles denote experimental values.\(^1\)
Figure 30: Radial distribution of Reynolds averaged mixture fraction $\langle Z \rangle_L$, total $RMS(Z)$ and temperature $\langle T \rangle_L$ in SMA2 at $z = 20$ mm (left), $z = 50$ mm (middle) and $z = 100$ mm (right). The thick solid line denotes SMFDF predictions and the circles denote experimental values.\footnote{1}
Figure 31: Radial distribution of Reynolds averaged $\langle Y_{CO} \rangle_L$, $\langle Y_{OH} \rangle_L$, $\langle Y_{H_2O} \rangle_L$, and $\langle Y_{CO_2} \rangle_L$ in SMA2 at $z = 20$ mm (left), $z = 50$ mm (middle) and $z = 100$ mm (right). The thick solid line denotes SMFDF predictions and the circles denote experimental values.
4.0 FDF SIMULATION OF A REALISTIC GAS TURBINE COMBUSTOR

In the work described in this chapter, the unstructured S-FMDF methodology is extended to conduct LES of a realistic swirl flame combustor. This is the PRECCINSTA experimental burner from the German Aerospace Center (DLR).\textsuperscript{2} The PRECCINSTA burner is a reasonable representation of an industrial gas turbine combustor and has been the subject of broad experimental\textsuperscript{2} and computational\textsuperscript{67-70} investigations. To keep the geometrical complexity of the burner intact, the fuel injection holes are meshed along with radial swirler vanes and the mixing zone prior to the nozzle exit. Two flame conditions are considered in the experiment. The first is an unsteady pulsating flame at a global equivalence ratio of 0.7, and the second is a quiet flame at a global equivalence ratio of 0.83. The latter flame is the subject of LES in this chapter. The simulated data are analyzed by comparison of the Reynolds-averaged statistics with experimental data and show excellent agreements. This demonstrates the capability of FDF for LES of complex flows, and warrants future applications of the methodology for LES of practical combustor configurations.

4.1 FLAME CONFIGURATION

The schematic of the PRECCINSTA burner\textsuperscript{2} is shown in Fig. 32. It features a plenum, a swirler, a square combustion chamber and a cylindrical exhaust pipe. Dry air at ambient temperature is fed via the plenum (diam. 78 mm) through radial swirler vanes to the burner nozzle. The fuel gas (CH\textsubscript{4}) is injected into the air flow through 12 small holes within the radial swirler with high momentum to ensure good mixing before entering the combustion chamber. This chamber consists of large quartz windows of 1.5 mm thickness held by steel posts in
the corners, thus creating a confinement with a square cross section of 85 mm × 85 mm, and a height of 114 mm. The exit of the upright combustion chamber is conically shaped leading to a short central exhaust pipe with a contraction ratio of approximately \( \frac{1}{5} \). A central conical hub upstream of the combustion chamber stabilizes and controls the position of the flame. The total mass flow rate into the burner is 12.9 g/s. Quantitative measurements of major species and temperature are provided in vertical planes at eight different cross-sections downstream of the injector. The statistical uncertainties are less than 2.5% and 7% respectively for temperature and most species except for CO and H\(_2\) where it is between 20 – 50%.

Combustion chemistry is modeled via the augmented reduced mechanism (ARM) of Sung et al.\(^{71}\) This is derived from GRI-Mech 1.2 for methane oxidation and it features 16 species and 12 reaction steps. The ISAT algorithm\(^ {64} \) is employed for the kinetics simulations.

4.2 RESULTS

The mesh topology for the PRECCINSTA burner is shown in Fig. 33. It consists of 2.2 million tetrahedral unstructured mesh elements. The fuel and the air inlet mass flow correspond to the case of quiet combustion examined by DLR\(^2\) with a global equivalence ratio of 0.83. Fresh gases are injected at 320 K and the walls of the combustor are assumed adiabatic. The S-FMDF solver is initialized with 30 particles per cell. The particles are supplied at the inlets and move within the domain due to the combined actions of convection and diffusion (molecular and SGS). During the course of simulations, the total number of particles within the domain is about 66 million. The simulations are conducted for 8 flow-through times. The results are monitored to ensure that the particles fully encompass and extend well beyond regions of non-zero vorticity and reaction. The Reynolds-averaged statistics, to be compared with experimental data,\(^2\) are obtained by long time (5 flow-through times) averaging of the filtered values. The notations \( \overline{Q} \) and \( \text{RMS}(Q) \) denote the Reynolds-averaged mean and the root mean square values of the variable \( Q \), respectively. For the RMS, the contributions of both the resolved and the subgrid counterparts are included.
Figure 34 shows the contour plot of the instantaneous filtered temperature field on the left and a snapshot of the filtered temperature iso-surface on the right. Figure 35 shows the volume rendered, instantaneous CO mass fraction. The flame with a V-shape is located near the burner inlet and shows wrinkling in its structure. The flame extent is short and combustion is observed to be almost over by about 36 \text{mm} from the central conical head. The flow pattern in the PRECCINSTA burner shows a complex structure with a toroidal recirculation zone at the base of the central conical body. Recirculation is also observed in the corners of the combustion chamber. Figure 36 shows the streamline pattern of the flow on a central plane based on the Reynolds-averaged mean velocities. The toroidal structure of the turbulent flow is further evident in the iso-surface of the second invariant of the velocity deformation tensor colored by temperature as shown in Fig. 37.

The capability of S-FMDF in predicting the PRECCINSTA flame is demonstrated by examining the transverse profiles of the mean and the RMS temperature values at seven axial locations in Figs. 38 and 39, respectively. These figures indicate that the predicted values agree quite well with experimental data. The statistics of the mass fractions of some of the species (CO\textsubscript{2}, CO) are compared with experimental data in Figs. 40-43, and again show good agreements. The mean CO is slightly over-predicted. However, the experimentally measured values portray about 50\% error in the measurement of CO.

4.3 CHAPTER SUMMARY

The unstructured scalar filtered mass density function (S-FMDF) methodology is employed for LES of the PRECCINSTA burner from DLR.\textsuperscript{2} The predictive capability of the model is assessed by comparison of the Reynolds-averaged statistics of the thermo-chemical variables with measured data. In general, excellent agreements are observed. This demonstrates that FDF can now be considered for LES of flames in practical combustors.
Figure 32: Schematic of the PRECCINSTA burner\(^2\) and the combustion chamber.
Figure 33: Tetrahedral mesh on the PRECCINSTA burner\(^2\) and the combustion chamber.
Figure 34: Left: Instantaneous temperature plot on a central plane, Right: Instantaneous 1200 K iso-surface of the filtered temperature field.
Figure 35: Instantaneous volume rendered plot of CO mass fraction.
Figure 36: Reynolds-averaged velocity-based streamline pattern on the central plane showing recirculation zones.
Figure 37: Flow structure for PRECCINSTA burner\textsuperscript{2} visualized by iso-surface of the second invariant of the instantaneous velocity deformation tensor colored by the filtered velocity.
Figure 38: Transverse distribution of Reynolds averaged temperature, $\langle T \rangle_L$ in the burner at several axial distances. The thick solid line denotes SMFDF predictions and the circles denote experimental values.\textsuperscript{2}
Figure 39: Transverse distribution of Reynolds averaged RMS temperature, $\overline{RMS(T)}$ in the burner at several axial distances. The thick solid line denotes SMFDF predictions and the circles denote experimental values. ²
Figure 40: Transverse distribution of Reynolds averaged $\langle CO_2 \rangle_L$ in the burner at several axial distances. The thick solid line denotes SMFDF predictions and the circles denote experimental values.\textsuperscript{2}
Figure 41: Transverse distribution of Reynolds averaged \( \overline{RMS(CO_2)} \) in the burner at several axial distances. The thick solid line denotes SMFDF predictions and the circles denote experimental values.\(^2\)
Figure 42: Transverse distribution of Reynolds averaged $\langle CO \rangle_L$ in the burner at several axial distances. The thick solid line denotes SMFDF predictions and the circles denote experimental values.²
Figure 43: Transverse distribution of Reynolds averaged $\overline{RMS(CO)}$ in the burner at several axial distances. The thick solid line denotes SMFDF predictions and the circles denote experimental values. ²
5.0 CONCLUSIONS

The filtered density function (FDF) methodology has proven very effective for large eddy simulation (LES) of turbulent reactive flows. In almost all previous investigations, FDF simulations have been conducted on structured meshes. This has restricted its applicability to simple configurations. The objective of this dissertation is to extend the applicability of FDF to unstructured meshes in order to widen its use for LES of realistic combustors. The implementation is done via the commercial CFD code ANSYS FLUENT.\textsuperscript{35}

First, some new tools are developed to facilitate FDF implementation on unstructured grids. They include an efficient algorithm to track particles and a new “basis function method” scheme to evaluate particle statistics on unstructured grids. Detailed error estimates are provided for this scheme. The overall capability of the unstructured FDF simulator is assessed via LES of a temporally developing turbulent mixing layer under both non-reacting and chemically reacting conditions. The consistency and realizability of the simulated results are established and the predictive capability of FDF is demonstrated via comparison with direct numerical simulation (DNS) data.

Next, the unstructured FDF methodology is employed for LES of two swirl stabilized non-premixed flames.\textsuperscript{1} These are low-swirl (SM1) and high-swirl (SMA2) methane flames; both of which have been the subject of detailed laboratory measurements. Combustion chemistry is modeled via a flamelet model for SM1, and a detailed finite rate kinetics model for SMA2. The simulated results are assessed via comparison with experimental data and show excellent agreements.

Finally, the methodology is extended to conduct LES of a realistic gas turbine combustor, the PRECCINSTA experimental burner from the German Aerospace Center (DLR).\textsuperscript{2} The simulated results are again assessed via comparison with experimental data and show excel-
lent agreements. This demonstrates the capability of the unstructured FDF solver for LES of complex flows in realistic geometries, and warrants future applications of the methodology for LES of practical combustor configurations.

Some suggestions for possible future work are:

- Development of a stochastic FDF formulation on unstructured grids to include the velocity and the mixing frequency. In the current FDF implementation, the velocity field is obtained by the finite-volume solver, and the mixing frequency is modeled in an *ad hoc* manner. The VS-FMDF\textsuperscript{7,8} and FVS-FMDF\textsuperscript{6} would make excellent candidates for future simulations on unstructured grids.

- Introduction of a stochastic model on unstructured grids suitable for high Mach number flows. To account for the effects of compressibility, the system of stochastic differential equations (SDEs) must include additional thermodynamical variables such as pressure and internal energy.\textsuperscript{72,73}

- Inclusion of differential diffusion effects.\textsuperscript{74–79}


