Large Eddy Simulation of Turbulent Combustion via Filtered Mass Density Function

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This paper provides a brief review of the scalar filtered mass density function (FMDF) model. The FMDF is a subgrid-scale probability density function (PDF) model for large eddy simulation (LES) of turbulent combustion and is obtained by the solution of a set of stochastic differential equations by a Lagrangian Monte Carlo method. The applicability and the validity of the LES/FMDF are established by simulating various low and high speed, single- and two-phase turbulent reacting flows. The LES/FMDF results are found to be consistent and comparable to DNS and experimental results for different flows.

I. Introduction

The efficiency and stability of combustor in advanced propulsion systems is controlled by various parameters such as the input/output flow conditions, the geometry, the fuel type, the equivalence ratio and the fuel-air premixing. Normally, it is very difficult to predict the flow in the combustor under various operating conditions and it is extremely costly and time consuming to develop a new combustor just by experimentation. On the other hand, high fidelity computational models are relatively inexpensive and could provide valuable, detailed, time-dependent spatial data. One of the high fidelity models that are becoming more popular for the development of compact and efficient combustors is the large-eddy simulation (LES).

Despite its great potential, LES is not fully utilized for the development of new combustion systems due to challenges in subgrid-scale (SGS) modeling and numerical implementation of LES. In particular, modeling and numerical simulations of high speed and multiphase reacting flows have proven to be very difficult. A major challenge is to develop affordable models which can properly describe the complicated interactions among turbulence, combustion, phases and shockwaves at a wide range of time and length scales. This paper describes how to solve LES for turbulent combustion based on a hybrid Eulerian-Lagrangian mathematical/computational methodology. The Eulerian part of the model employs a generalized high-order finite-difference method for the solution of compressible velocity field and is applicable to both subsonic and supersonic turbulent flows in complex geometries. The subgrid mixing and combustion are computed with a PDF-based model, termed the filtered mass density function (FMDF) and a Lagrangian Monte Carlo method\(^1\). The FMDF was originally developed for low Mach number single-phase reacting flows. Recently, we have extended the model to compressible flows and sprays and have successfully tested it for various problems. The LES/FMDF is found to be able to capture the interactions among turbulence, combustion and spray, and has shown to be applicable to a variety of turbulent flames\(^1\).\(^5\)

II. Filtered Mass Density Function (FMDF)

In “conventional” LES methods, the “resolved” field is obtained by solving the filtered form of the compressible Navier-Stokes, energy and scalar equations\(^5\). The filtered equations are closed via appropriate SGS stress and scalar flux models. In reacting flows, additional models are required for the reaction source/sink terms. Here, we use the FMDF which has been implemented in two ways: (Formulation I) to consider only the SGS scalar quantities\(^1\), and (Formulation II) to consider the SGS velocity-scalar-(pressure) quantities\(^7\). Formulation I is more manageable

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computationally, and formulation II is more rigorous from the statistical standpoint. Most of our previous contributions are based on formulation I, which is more suitable for simulations of practical combustion systems.

Earlier applications of the FMDF/FDF model (FDF or filtered density function is the constant-density version of the FMDF) were for relatively simple, fundamental mixing and combustion problems and were focused on the development and testing of the model for low-speed single-phase flows. The scalar FDF was considered in Refs. 8,9, the scalar FMDF in Refs. 1,5,10–11, the velocity FDF in Ref. 7, the velocity–scalar FDF in Ref. 12 and the velocity-scalar FMDF in Ref. 13; a review of these works is provided in Ref. 14.

With the advancements in computational power and with the development of more efficient parallel numerical algorithms for the hybrid Eulerian-Lagrangian equations, the FMDF model has been used for the simulations of increasingly more sophisticated flows over the past several years. These simulations have been conducted in conjunction with non-equilibrium and equilibrium reaction models and reduced and detailed chemical kinetics mechanisms for various non-premixed, partially-premixed and premixed turbulent flames. Several applications of the low-speed scalar FMDF model to turbulent jet flames have been reported. Sheikhi et al. 15, Raman and Pitsch 16 and Yaldızlı et al. 17 employed the scalar FMDF for LES of Sandia’s partially-premixed methane jet flames with complex chemical kinetics mechanisms, using the flamelet assumption or direct finite-rate chemistry solver. The velocity-scalar FMDF is also used for the simulations of Sandia’s jet flames 18. Experiments were conducted for several turbulent jet speeds. For the lowest jet speed considered (the so called flame D), the flame was burning near equilibrium with limited local extinction. For this condition, the scalar FMDF results as obtained with the flamelet model and detailed mechanisms were found to be close to the experimental data. However, for the higher jet speeds (flames E and F), with significant local extinction, the flamelet model fails to reproduce the experimental data. In contrast the LES/FMDF with finite-rate multi-step reaction mechanisms was shown to be able to predict “high speed” flames E and F. The effects of SGS turbulence and mixing models are shown to be more important in high speed flames when finite-rate chemistry effects are more important.

Afshari et al. 19 used the scalar FMDF to simulate a premixed propane-air flame in an axisymmetric dump combustor. A density-based, multi-block flow solver has been used for the solution of filtered continuity, momentum, and energy equations with various subgrid turbulence closures. All spatial derivatives are approximated by high-order compact differencing and time derivatives are modeled via a low-storage, three-stage, and third-order Runge-Kutta scheme. For the Lagrangian Monte Carlo solution of the FMDF over complex multiblock, but structured, grid systems, new parallel particle interpolation and search algorithms were used. Consistency between the Eulerian (finite difference) and Lagrangian (Monte Carlo) parts of the hybrid LES/FMDF model indicates that the model is numerically accurate. Additionally, the LES/FMDF predictions were found to be close to the experimental data. A novel irregular Monte Carlo portioning procedure that facilitates the efficient parallel implementation of complex kinetics in the FMDF was used by Yilmaz et al. 20 for simulating a methane Bunsen-Burner flame with a 5-step, 9-species mechanism.

In the previous applications of the LES/FMDF, the effect of pressure on the scalar FMDF or the velocity-scalar FMDF was not considered. This effect could be ignored at low Mach number flows or constant pressure combustion. However, it is important and should be included in the FMDF for compressible (subsonic or supersonic) flows or combustion in closed systems such as the internal combustion engines. Compressibility effect can be implemented in the scalar and velocity-scalar formulations of the FMDF both. In the later formulation, the pressure and energy are coupled with the velocity, temperature, density and species mass fractions; therefore are included in the definition of the joint FMDF and its transport equation. The joint energy-pressure-velocity-scalar-FMDF is the most complete and complex formulation of the FDF that has been ever considered 21. However, it is still under developed and cannot be used for simulations of a practical combustion system. In the compressible scalar formulation of the FMDF, the FMDF involves the scalars and the energy and not the velocity or pressure. In this formulation, the compressibility terms are included via source terms added to the energy equation 22. The compressible scalar formulation of the FMDF is much more manageable computationally, but the energy-pressure-velocity-scalar-frequency formulation is more rigorous from the mathematical/statistical standpoint. At this time, the scalar FMDF model is the only version of FMDF available for high speed turbulent reacting flows. To include the compressibility effects as observed in high speed flows at SGS level in our simulations via scalar FMDF, we follow an approach somewhat similar to those proposed by Hsu et al. 23 for RANS. In this approach, the conditional expectation of the material derivative of the pressure as appears in the enthalpy equation is added to the joint scalar FMDF equation. The effects of SGS pressure fluctuation on the density are neglected in the scalar FMDF method. The new model has been used for LES of several non-reacting and reacting compressible turbulent flows. Our results indicate that the new compressible scalar FMDF model is accurate and applicable to supersonic combustion systems.

2
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From a methodological point of view, the numerical methods that have been developed for two-phase turbulent flows are generally based on three different approaches: (i) Eulerian-Eulerian approach 25-27, (ii) Eulerian-Lagrangian approach 28-31, and (iii) Lagrangian-Lagrangian approach 32-33. In the first approach, the continuum transport equations for both phases are solved. These equations are somewhat similar and are often obtained by some sort volume averaging which is conceptually different than the ensemble averaging in RANS or space averaging in LES. In the second approach, the continuum carrier fluid equations are solved in its “instantaneous” form in DNS or its “averaged” form in RANS and LES over an Eulerian grid system. However, the “dispersed” (droplet) phase is described by a set of modeled Lagrangian equations which determine the position, velocity, temperature, and other properties 34-35 of the dispersed phase. In the third approach, both phases are described in the Lagrangian context. Despite significant progress that has been made in LES of two-phase turbulent flows, the application of LES to turbulent spray combustion or non-isothermal two-phase flows with evaporating/reacting droplets is somewhat limited 30,36. Among the limited number of LES studies on turbulent spray combustion, we refer here to the papers by Okong’o et al. 37, Leboissetier et al. 38, Sankaran et al. 39, Patel et al. 40, Mahesh et al. 41, Cuenot et al. 42 and Li et al. 43-44. Models used in these studies are mostly based on the Eulerian-Lagrangian approach in which the carrier gas equations are solved over fixed grid points but the spray is simulated with Lagrangian evaporating/reacting droplets. The combustion is often simulated with a flamelet/progress variable reaction submodel or similar models. The two-phase reacting LES model of Cuenot et al. 42 is fundamentally different than the Eulerian-Lagrangian models as it solves the Eulerian equations for both phases.

Recently, the scalar FMDF model and its numerical solution method are extended to two-phase reacting flows and are applied to turbulent spray combustion 43-44. A new mathematical/computational methodology is developed for the LES/FMDF, in which the liquid spray and FMDF equations are solved with Lagrangian methods, while the gas dynamic variables are computed by a “conventional” Eulerian method. The new multiphase LES/FMDF methodology was implemented through an efficient Lagrangian-Eulerian-Lagrangian computational model 43-44, and was applied to complex flows such as those occur in internal combustion (IC) engines 35. In this model, the filtered compressible Navier-Stokes equations are solved in a generalized curvilinear coordinate system with high-order, multi-block, compact and monotonicity-preserving finite-difference schemes for the turbulent velocity and pressure. However, the subgrid combustion is modeled with the two-phase scalar FMDF and its Lagrangian Monte Carlo solver. 43-45. A Lagrangian mathematical/computational method is used for the spray in which the evolutions of the droplet displacement vector, the droplet velocity vector, the droplet temperature and mass are described by a set of non-equilibrium Lagrangian equations 46. The two-way mass, momentum, and energy coupling between phases are implemented through several source/sink terms. The new two-phase LES/FMDF model is described more below together with some sample results.

### III. Sample Results

The scalar FMDF model has been used for the numerical simulations of various subsonic turbulent flames. These include Sandia’s partially-premixed piloted turbulent methane jet flames D and F 47. Flame D involves limited regions of local extinction, while flame F tends towards total extinction. The geometrical configurations in these two flames are the same, but the jet velocity in flame F is twice of that in flame D. The existence of different levels of local extinction in these flames provides a good means of assessing the capabilities of the models to predict realistic combustion systems. Figure 1 shows the LES/FMDF predicted ( Favre time-averaged) mean and root mean square (rms) values of the temperature, and species mass fractions in flames D and F as a function of the mean mixture fraction in comparison to the experimental data. The computed data are obtained by a 12-step reduced chemistry model. For flame D, both the peak and the shape of scalar and temperature profiles are well predicted by the LES/FMDF (Fig. 1a). At axial location of x/D=15, the rms of temperature appears to be slightly underpredicted. Considering the highly sensitive and oscillatory behavior of flame F, the mean and RMS of temperature are well predicted by the LES/FMDF (Fig. 1b) for this flame. The rms of temperature for flame F exhibits similar trend to that for flame D. It is also shown in Fig. 1c and d that the mean mass fractions of CO and H2 are well predicted for both flames at x/D=15. However, the CO profiles for flame F at x/D=7.5 (not shown) are found to be slightly different than experiment on the rich side of the flame (not shown), mainly due to finite rate effects. This is consistent with the underpredictions of the CO mass fraction in the rich side of the flame that has been reported in the literature 48.

As mentioned above, the LES/FMDF model has also been applied to high speed flows. One of these flows is an isotropic turbulent flow in a shock “tube.” The initial condition for the thermodynamic variables is based on Sod’s shock tube solution. However, unlike the Sod’s problem, the initial flow is an isotropic turbulent flow with intensity of 6 per cent of the laminar shock upstream velocity. Also, the flow is homogeneous and periodic in directions

3

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perpendicular to the shock/flow. Figure 2 shows the iso-levels of instantaneous filtered density as obtained by the finite difference (FD) LES and Monte Carlo (MC) FMDF parts of the hybrid LES/FMDF model for the shock-turbulence problem. Evidently, the shock wave has a significant effect on the turbulence. Nevertheless, the LES-FD and FMDF-FD predictions are shown to be consistent, even in the vicinity of the shock wave, indicating the ability of the compressible scalar FMDF model to capture the shock wave effects on the turbulence.

Figure 3 shows the grid and the vorticity contours in a coannular supersonic helium-air jet, which is also considered for the testing of compressible scalar FMDF model. The geometry is axisymmetric and consists of a central and an outer concentric annular nozzle passage. The gas jet at the central-nozzle inlet is the helium and the outer co-flow is air. This flow has been experimentally and numerically with the RANS models. We have simulated the flow with the LES-FD and FMDF-MC parts of the hybrid LES/FMDF model. The pressure and viscous dissipation terms are included in the FMDF equation. Contours of instantaneous scalar mass fraction as obtained from the FD and MC data are shown in Fig. 4. Qualitatively, LES-FD and FMDF-FD predictions are consistent in this supersonic problem. The time-averaged values of helium-oxygen mass fraction and temperature in Fig. 5 also indicate that the LES-FD and FMDF-MC predictions are consistent. Additionally, the computed mean and rms of the resolved helium-oxygen mass fraction and temperature by the FMDF-MC and LES-FD (not shown) are in good agreement with each other; further indicating the consistency and the reliability of the LES/FMDF model for supersonic turbulent flows. It is to be noted here that the LES-FD and FMDF-MC predictions deviate noticeably when the pressure term is removed from the FMDF formulation. The LES/FMDF predictions of the filtered scalar mass fraction are also found to be in good agreement with the experimental data.

For further assessment of LES/FMDF and its sub-models, simulations of complex two-phase reacting turbulent flows have also been conducted. Here we show some sample results for a double-swirl burner. Figure 6 shows the instantaneous vorticity iso-surfaces, the two-dimensional contours of filtered temperature and the radial (r) variations of temperature and fuel mass fraction as obtained by the FD and MC parts of the hybrid LES/FMDF model at two different axial (z) locations in the double-swirl spray burner. Evidently, the FD and MC results are very similar. The consistency of LES-FD and FMDF-MC results for the temperature and species mass fractions in this flow and other complex flows (e.g. the in-cylinder flow involving moving piston and valves, spray, droplet evaporation, mixing, flame ignition and propagation) indicates the numerical accuracy and the practicality of the LES/FMDF model. The results obtained with the LES/FMDF for a variety of single-phase, two-phase, low speed and high speed flows are also found to compare well with the DNS and available experimental data.

References


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**Figure 1.** Comparison between LES/FMDF and experimental data in the mixture fraction space for the 12-step model at x/D=15: (a) mean temperature, rms of temperature and mean O2 mass fraction for flame D; (b) mean temperature, rms of temperature and O2 mass fraction for flame F; (c) mean CO and H2 mass fractions for flame D; (d) mean CO and H2 mass fractions for flame F. Lines represent LES/FMDF results and symbols represent experimental results.
Figure 2. Instantaneous iso-levels of the filtered density obtained by LES-FD and FMDF-MC.

Figure 3. Two- and three dimensional grids and contours of the vorticity magnitude in the supersonic coannular helium-air jet.

Figure 4. Instantaneous contours of the scalar mass fraction predicted by the LES-FD, FMDF-MC.
Figure 5. Comparison of the time-averaged $He-O_2$ mass fraction and filtered temperature, obtained with the LES-FD model (solid lines), (dashed dot lines) and FMDF-MC model (dashed-dot lines with hollow symbols) with the experimental data (solid symbols). (a) $He-O_2$ mass fraction. (b) Filtered temperature. $T_{ref}=300K$.

Figure 6. Instantaneous vorticity iso-surfaces, two-dimensional contours of filtered temperature and the radial ($r$) variations of temperature and fuel mass fraction as obtained by the finite difference (FD) and Monte Carlo (MC) parts of the hybrid LES/FMDF model at two different axial ($x$) locations in the double-swirl spray burner.