Consistent hybrid LES-FDF simulation of turbulent reactive flows

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Abstract

A hybrid large-eddy simulation/filtered-density function (LES-FDF) scheme is devised and implemented for the simulation of turbulent reactive flows. A robust validation criteria is specified in terms of the moments of the FDF transport equation. By using redundant quantities in the different components of the hybrid-solver, a consistency condition is specified. For the current joint-composition FDF-based method, the density field is used as the redundant field. The consistency criteria is tested using a complex bluff-body stabilized flame.

Keywords: Combustion; Turbulent flow; Large-eddy simulation; Filtered-density function; Monte-Carlo scheme; Hybrid approach

1. Introduction

Simulation of turbulent reactive flows is a complex and challenging problem with widespread practical use. Recent breakthroughs in algorithmic techniques and the drastic increase in computing power have provided us with the tools to understand the complex interaction between turbulence and chemical reaction. In the past decade, use of the large-eddy simulation (LES) technique has made it possible to make accurate predictions of turbulent flow even for complex configurations. On the other hand, treatment of combustion is mainly through simple closures and pre-existing models from the Reynolds-averaged Navier–Stokes methods (RANS) such as flamelet models or conditional moment closure type approximations. Although these assumptions work well for systems that exhibit little or no extinction, a higher-dimensional multi-scalar model is required to describe slow and extinction chemistry. The transported-filtered density function (FDF) [1] method provides a natural starting point for such detailed description. The FDF technique has the key advantage that the reaction source term of the scalars appears closed and requires no modeling.

Though a joint velocity-composition FDF transport equation can be formulated, numerical implementations of this high-dimensional system pose stability and feasibility issues. To overcome this problem, a hybrid approach is used where the velocity and turbulence fields are solved using an Eulerian scheme (like RANS or LES) while the scalar transport is handled using the FDF approach. Although the FDF technique has been widely used in the RANS context, almost all the applications involve steady-state flows. Since the LES technique is inherently transient, the coupled LES-PDF method needs to maintain temporal accuracy. Due to the statistical nature of the FDF scheme, such a coupled scheme poses numerical accuracy issues. This article details a stable, robust and accurate formulation of the hybrid approach.

2. Hybrid LES-FDF scheme

In the hybrid scheme implemented here, the LES technique is based on a low-Mach number approximation-based finite-volume scheme. Further details of the LES implementation can be found elsewhere [2]. The Lagrangian method uses stochastic particles to evolve the FDF.

The particle method is obtained from the fundamental FDF transport equation. The FDF in a variable density flow can be defined as

$$F_L(\boldsymbol{\psi};\mathbf{x},t)=\int_{-\infty}^{+\infty}\rho(\mathbf{y},t)\,\xi[\boldsymbol{\psi},\boldsymbol{\phi}(\mathbf{y},t)]\,G(\mathbf{y}-\mathbf{x})\,d\mathbf{y} \tag{1}$$

$$\xi[\boldsymbol{\psi},\boldsymbol{\phi}(\mathbf{y},t)]=\delta[\boldsymbol{\psi}-\boldsymbol{\phi}(\mathbf{y},t)] \tag{2}$$

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where δ is a N-dimensional delta function for a N-species system and $\boldsymbol{\psi}$ is the random variable in the composition domain. The FDF definition yields the following property:

$$\int_{-\infty}^{+\infty} F_L d\boldsymbol{\psi} = \int_{-\infty}^{+\infty} \rho(\mathbf{y},t)\, G(\mathbf{y}-\mathbf{x})\, d\mathbf{y} = \bar{\rho} \tag{3}$$

Similarly, the filtered mean of any scalar Q_ϕ can be defined as

$$\widetilde{Q}_\phi = \int_{-\infty}^{+\infty} Q_\phi(\boldsymbol{\psi},\mathbf{y},t) F_L d\boldsymbol{\psi} = \frac{1}{\bar{\rho}} \int_{-\infty}^{+\infty} \rho(\mathbf{y},t)\, Q_\phi(\mathbf{y},t)\, G(\mathbf{y}-\mathbf{x})\, d\mathbf{y} \tag{4}$$

Using these definitions, the transport equation for the joint composition FDF can be written as [1,3]

$$\frac{\partial F_L}{\partial t} + \frac{\partial}{\partial \mathbf{x}}(\tilde{\mathbf{u}} F_L) + \frac{\partial}{\partial \mathbf{x}}\left(\widetilde{\mathbf{u}'|\boldsymbol{\psi}} F_L\right) = -\frac{\partial}{\partial \boldsymbol{\psi}}\left[\left(\frac{1}{\bar{\rho}}\overline{\nabla\cdot\rho D\nabla\boldsymbol{\phi}|\boldsymbol{\psi}} + \mathbf{S}(\boldsymbol{\psi})\right) F_L\right] \tag{5}$$

where $\tilde{\mathbf{u}}$ is the filtered velocity field, $\widetilde{\mathbf{u}'|\boldsymbol{\psi}}$ is the sub-filter velocity fluctuation conditioned on the scalar, $\overline{\nabla\cdot\rho D\nabla\boldsymbol{\phi}|\boldsymbol{\psi}}$ is the conditional micromixing term, and $\mathbf{S}$ is the reaction source term. The conditional velocity term is modeled using the gradient-diffusion hypothesis to give

$$\widetilde{u_i'|\boldsymbol{\psi}} F_L = -\bar{\rho} D_T \frac{\partial F_L/\rho}{\partial x_i} \tag{6}$$

The conditional mixing term is closed using the Interaction-by-Exchange-with-the-Mean (IEM) model [4]:

$$\overline{\nabla\cdot\rho D\nabla\boldsymbol{\phi}|\boldsymbol{\psi}} = \nabla\cdot\bar{\rho} D\nabla\tilde{\boldsymbol{\phi}} - \frac{\bar{\rho} C_\phi}{\tau}\left(\boldsymbol{\psi} - \tilde{\boldsymbol{\phi}}\right) \tag{7}$$

where C_ϕ is scalar-to-mechanical time-scale ratio and τ is a turbulence time scale. In the present study we set C_ϕ to be 2 [5] and use a turbulent-diffusivity-based time scale [1].

The high dimensionality of the FDF equation makes finite-differencing-based solution techniques infeasible. A stochastic approach [6] is used where the filtered momentum equations are solved using conventional grid-based techniques (like LES) while the FDF equation is solved using a particle-based Monte-Carlo approach. The Lagrangian system uses the filtered fields from the LES solver to advance the notional particles. Using the particle properties, mean fields are constructed that is fed back to the LES solver. The LES solver then advances the flow using these mean fields. Typically, the Lagrangian system provides the filtered density field that is then used by the LES solver.

To increase statistical accuracy, large particle numbers are needed making such methods computationally expensive. Numerical implementation of the LES-FDF scheme is an algorithmic challenge and novel techniques are used to reduce the computational expense of these schemes [7]. A major issue in such implementations is to consistently couple a stochastic FDF scheme and a deterministic Eulerian scheme. Although steady-state-based flow solvers have been successfully used [8], a consistent algorithm for a temporally variant system (like the LES-based approach) has not been studied in detail so far. Here we propose a criteria for a consistent implementation and test it with a challenging reacting flow problem.

3. Consistency requirements

In the Lagrangian particle-based system, the computational domain is decomposed into a large number of notional particles that represent the fluid. The particles are initially distributed uniformly and evolve in space and time using stochastic differential equations [6]. Each particle carries information about its location, a composition vector and a representative weight. In order to pass information from and to the LES solver, particle mean fields are obtained by a weighted summation process involving particle properties in a given computational cell. The particle weight is initially assigned to be the local fluid mass such that the sum of the particle weights in a computational cell equals the cell fluid mass:

$$w_k = \frac{V_i \bar{\rho}_i}{N_p} \tag{8}$$

where w_k is the particle weight, V_i is the cell volume, $\bar{\rho}_i$ is the fluid density in cell i, and N_p is the number of particles in the cell. At any time step, the particle-weights-based density can be obtained by using the sum of particle weights in a given cell:

$$\bar{\rho}_w = \frac{1}{V_i}\sum_{i=1}^{N_p} w_k \tag{9}$$

In addition to the particle weight, a mean density can also be obtained from the particle composition vector based on thermochemical properties:

$$\bar{\rho}_p = \frac{\sum_{k=1}^{N_p} w_k/\rho(\phi_k)}{\sum_{k=1}^{N_p} w_k} \tag{10}$$

where $\rho(\phi)$ is the thermochemical density computed using the particle composition. The initial conditions are chosen such that $\bar{\rho} >= \bar{\rho}_p$ at $t = 0$. As the particles evolve in space and time, the density fields evolve through different equations, though indirectly, they

should all satisfy the continuity equation. By construction [7], the thermochemical density ($\bar{\rho}_p$) and the LES density ($\bar{\rho}$) evolve closely. This is ensured by solving an ancillary enthalpy transport equation using Eulerian schemes. The source term for the enthalpy equation is provided using the particle properties. The Eulerian density is obtained directly using this enthalpy field [8].

On the other hand, the particle-weights-based density ($\bar{\rho}_w$) evolves with the particle motion. Based on the continuity equation, it can be shown [6] that for the particles to be uniformly distributed, the particle-weights-based density should be equivalent to the Eulerian density field. However, the stochastic evolution scheme will make the particle-based mean fields noisy. Hence a strict equality can be obtained only by time-averaging a statistically stationary field. Finite particle number density can also introduce bias in the mean fields. This will lead to a progressive divergence of the particle-weights-based density field from the Eulerian field. Such a bias will be readily observed through particle agglomeration in certain sections of the grid and depletion of particles in other regions. The sampling error induced by such low particle number density will further increase the error in mean-field estimation.

A consistent algorithm should hence maintain the equivalence of the three density fields described above. It is noted that this amounts to a consistent evolution of the zeroth moment of the FDF-transport equation. The accuracy of the scheme can be tested using higher-order moments of the same equation. For the single-scalar flamelet model used here, the first moment of the scalar can be evolved simultaneously by both the particle and Eulerian systems. Such a moments-based validation procedure ensures a robust yet simple way of demonstrating the accuracy of the numerical implementation. We illustrate the validation criteria using an experimental flame next.

4. Numerical test

A bluff-body stabilized experimental flame is simulated using the LES-FDF scheme. The methane/hydrogen fuel jet is separated from the coflow of air by a solid body (Fig. 1). The presence of this bluff-body induces strong recirculation zones that stabilize the flame. In fact, time-averaged streamtraces (Fig. 2) show the presence of two counterrotating vortices that help mix the coflow with the fuel. The interaction of the high-velocity jets with the slow recirculating fluid creates high shear rates where the reaction is controlled predominantly by mixing. This complex unsteady reacting flow makes an ideal candidate for testing the LES-FDF scheme. A computational domain of $256 \times 128 \times 32$ is used along with a nominal particle number density of 15. Combustion is described using a laminar flamelet chemistry. Further details of the simulation and the experimental configuration can be found in [7].

Figure 3 shows time-averaged radial profiles of the three density fields. The density profiles show excellent agreement indicating that the FDF implementation is accurate. It was further confirmed that the time-averaged particle number density was constant indicating

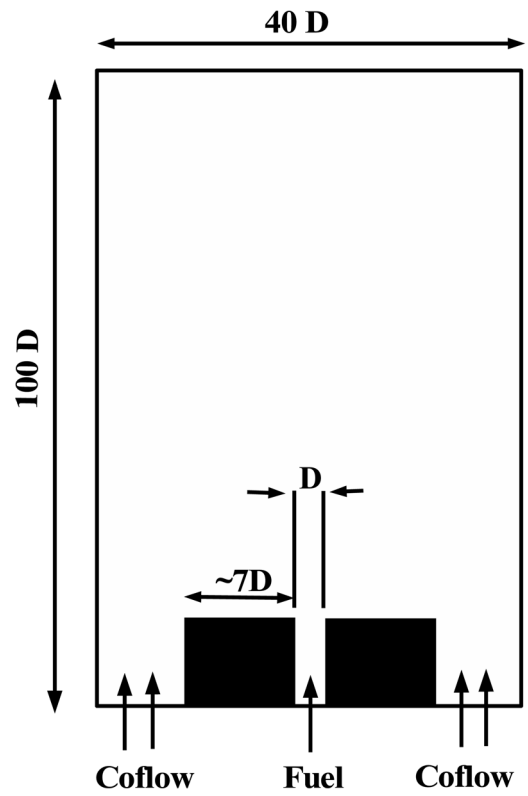

Fig. 1. Schematic of the bluff-body flame configuration. The jet diameter D is 3.6 mm.

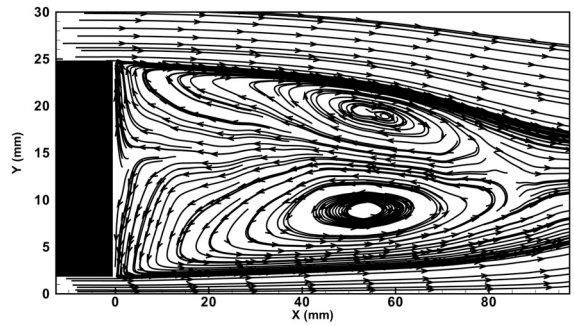

Fig. 2. Streamtraces of the time-averaged velocity vector showing the counter-rotating vortices.

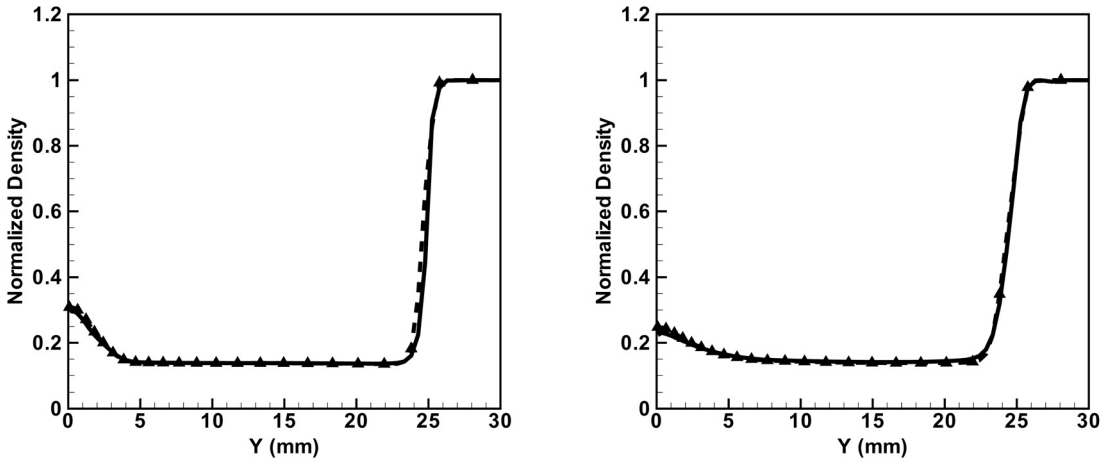

Fig. 3. Comparison of density obtained from particle weights (dashed line), particle composition (solid line) and LES flow solver (symbols). The plots are at downstream locations of (left) $x = 13$ and (right) $x = 30$ mm, respectively. The density values have been normalized by the density of the coflow.

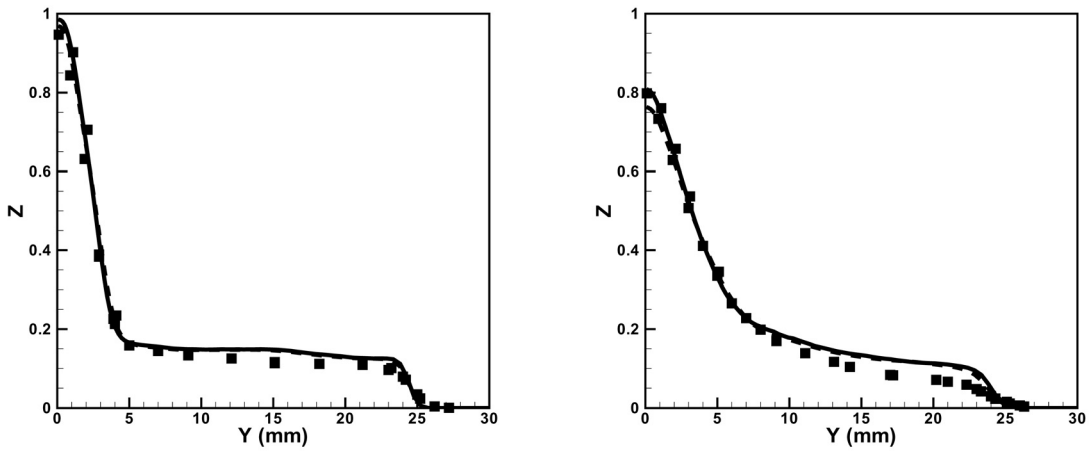

Fig. 4. Comparison of mean mixture fraction and RMS mixture fraction profiles with experimental data at different axial locations of (left) $x = 13$ and (right) $x = 30$ mm. Symbols are experimental data, solid line shows the FDF-based result and dashed line shows the Eulerian calculation.

that there was no long term accumulation of statistical errors. Figure 4 shows the comparison of the first moment of the scalar, namely time-averaged filtered mixture-fraction. Again the agreement between the Eulerian and Lagrangian fields is excellent. In addition, excellent agreement is noticed with experimental data as well illustrating the superior predictive capabilities of this method.

6. Conclusion

The LES-FDF scheme has been validated by using a density-based consistency condition. An experimental flame configuration was used to test the validation scheme. Currently, finite-rate chemistry is being used with a detailed chemical mechanism to fully exploit the advantages of the LES-FDF technique.

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