



Simulation of turbulent reactive flows using a FDF methodology – Advances in particle density control for normalized variables

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ABSTRACT

The present work is devoted to the development and implementation of a computational framework to perform numerical simulations of low Mach number turbulent reactive flows. The numerical algorithm designed for solving the transport equations relies on a semi implicit predictor-corrector integration scheme. The final computational model relies on a hybrid Large Eddy Simulation / transported Filtered Probability Density Function (FDF) framework. The TVD method CUBISTA is used in the discretization of the advective terms of the transport equations. The dynamic Smagorinsky turbulence closure model is retained and the influence of residual sub-grid scale scalar fluctuations on the filtered chemical reaction rate is taken into account within the Lagrangian PDF framework. The corresponding PDF model makes use of a Monte Carlo technique: Stochastic Differential Equations (SDE) equivalent to the Fokker-Planck equations are solved for the progress variable of chemical reactions. Due to the stochastic nature of the Monte-Carlo method and to the turbulent motions, the number of particles present in a given cell may significantly change in time. We present an algorithm for conservation of statistical moments up to second order and suggestion of how one may reduce drastically a notional particle population and yet maintain an acceptable PDF shape. The TVD algorithm capabilities are demonstrated in the one-dimensional advection of different pulses, the energy equation is validated through the simulation of a natural convection flow in a cavity. Finally, the new cloning and annihilation particles algorithm is tested on known (given) PDF functions and then applied to LES of reactive turbulent channel flows of methane/air mixtures.

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1. Introduction

Probability density function (PDF) methods offer compelling advantages for modeling chemically reacting turbulent flows [1,2]. In particular, they provide an effective resolution to the closure problems that arise from averaging or filtering the highly nonlinear chemical source terms, and other terms that correspond to one-point physical processes in the instantaneous governing equations [3]. The closure of the chemical source term represents a challenge, since the derived representations of the mean chemical source term must be consistent with known theoretical constraints and experimental observations, without the direct knowledge of sub-grid scalar fields. Indeed, such an information would be available in a DNS simulation, however, DNS simulations for turbulent reacting flows are not easily tractable with the present computational power. This characteristic implies that, in principle, even complex chemical kinetics schemes can be treated without closure difficul-

ties by a transported PDF-based method. Another reason is that statistical moments of first and second order, associated to RANS or LES models, can be easily evaluated. Due to its applicability and capacity in dealing with complex phenomena, the FDF method has been improved throughout the years [4–9]. Complex multi-physics and realistic (industrial) applications may be found, respectively in [10,11].

In contrast with classical algorithms that are commonly retained to perform the numerical simulation of a set of partial differential equations, i.e., finite-difference or finite-volume methods, the modeled PDF transport equation has a rather different structure. It is a high-dimensional scalar transport equation, and it is less amenable for finite-volume or finite-difference methods. From early on times in the development of PDF methods, Monte Carlo techniques, in which the PDF is represented by an ensemble of stochastic particles, have been employed [12]. Stochastic differential equations (SDEs) are constructed to model the particle properties, e.g., velocity, composition, and frequency, such that the particles exhibit the same PDF as in the turbulent flows.

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Due to the stochastic nature of the method of Monte–Carlo and to the turbulent motions, the number of particles present in a given cell may significantly change in time. In order to prevent particle accumulations in certain regions and an insufficient number of particles in others, it is crucial to have a mechanism of particle density control. In the present work we show results of an algorithm developed to ensure statistical moment conservation up to second and yet maintain the original PDF form of the particles distribution in a finite-volume cell. It is worth noting that the present work is the product of a fruitful scientific collaboration between the Fluid Mechanics Laboratory (MFLab) of the Federal university of Uberlândia and Petrobras S.A.

This paper is organized as follows: In Section 2.1 the mathematical modeling used in the present work is discussed for both Eulerian and Lagrangian approaches. Section 2.2 presents the essential features of the numerical solver *FLUIDS_3D*, including the Navier–Stokes, the TVD verification and Stochastic differential Equations solvers. Sections 2.3 and 2.4 report the novel proposal for particle density control for normalized variables. Section 3 discuss the validation of a version of an energy equation as well as its coupling with the Navier–Stokes Solver. It is worth noting that specifically in this section the Boussinesq approximation is used since the density variations are small compared to combustion applications that will be finally shown in Section 4. In this case, the coupling between the temperature and density variations are made by an equation of state.

2. Mathematical and computational modeling

The mathematical and computational framework retained to proceed with the numerical simulation is now briefly presented. The interested reader may find a detailed presentation elsewhere [13–15]. A hybrid approach in which the LES methodology is coupled with the transport of the scalar filtered probability density function (PDF) is retained to describe the reactive cases. The method involves the numerical solution of partial differential equations (LES solver) together with stochastic differential equations (PDF solver). From the LES approach the Eulerian filtered variables are evaluated, while stochastic differential equations (SDE) are solved using Lagrangian notional particles to simulate the modeled transport equation of the scalar PDF [1,12]. The latter yields the one-point, one-time statistics of subgrid-scale scalar fluctuations and thus provides the LES solver with the corresponding filtered chemical reaction rate.

2.1. Mathematical model

The present section is organized as follows: the filtered set of balance equations that describes the flows under consideration is first presented. The main characteristics of the transported FDF method are then briefly introduced together with the equivalent system of stochastic differential equations as well as the coupling between the Eulerian and Lagrangian approaches.

2.1.1. Set of filtered equations

The following simplifying assumptions are used: (a) fluid is considered as Newtonian, (b) body forces, heat transport by radiation, Soret and Dufour effects are not addressed, (c) the model is developed for low Mach number flows, (d) we consider unity Lewis number values and equal molecular diffusion coefficients for all species, (e) heat losses are neglected. The mathematical model considers multi-species variable-density reactive flows, in which the primary transported variables are the density ρ , the three velocity components u_i , the specific enthalpy h and the mass fractions Y_k of the K chemical species ($k = 1, \dots, K$), the balance equa-

tions are:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j}{\partial x_j} = 0, \quad (1)$$

$$\frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j \tilde{u}_i}{\partial x_j} = \frac{\partial \bar{T}_{ij}}{\partial x_j} - \frac{\partial \tau_{ij}^{SGS}}{\partial x_j}, \quad (2)$$

$$\frac{\partial \bar{\rho} \tilde{\phi}_\alpha}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j \tilde{\phi}_\alpha}{\partial x_j} = \frac{\partial \bar{Q}_{\alpha,j}}{\partial x_j} - \frac{\partial Q_{\alpha,j}^{SGS}}{\partial x_j} + \bar{S}_\alpha, \quad (3)$$

where the variable ϕ_α denotes the mass fraction of a chemical species or the enthalpy of the mixture, ($x_i, i = 1, 2, 3$) are the spatial coordinate, and t is the time. $T_{ij} = \tau_{ij} - p \delta_{ij}$ is the tensor of mechanical constraints including both a deviatoric (shear stresses τ_{ij}) and a spheric (pressure $p \delta_{ij}$) contribution, while $Q_{\alpha,j}$ denotes the component of the molecular diffusion flux of the scalar α in the direction j . In the above expression, $\tau_{ij}^{SGS} = (\bar{\rho} u_i \tilde{u}_j - \bar{\rho} \tilde{u}_i \tilde{u}_j)$ is the subgrid scale (SGS) stress tensor and $Q_{\alpha,j}^{SGS} = (\bar{\rho} u_i \tilde{\phi}_\alpha - \bar{\rho} \tilde{u}_i \tilde{\phi}_\alpha)$ represents the SGS scalar flux components, respectively. Finally, the last term in the RHS of Eq. (3), i.e. \bar{S}_α , denotes the filtered reaction rate. The above system is completed by an equation of state: $P = P_0(t) + p(\mathbf{x}, t)$, with $P_0(t)$ the thermodynamic pressure.

The unresolved momentum fluxes are expressed according to the Boussinesq assumption, $\tau_{ij}^{SGS} - \delta_{ij} \tau_{kk}^{SGS} / 3 = 2\mu_{SGS}(\tilde{S}_{ij} - \delta_{ij} \tilde{S}_{kk} / 3)$, where μ_{SGS} is the subgrid scale viscosity, and $\tilde{S}_{ij} = (\partial \tilde{u}_i / \partial x_j + \partial \tilde{u}_j / \partial x_i) / 2$ is the strain rate tensor of the resolved field [16,17]. The eddy viscosity μ_{SGS} is obtained from the Dynamic Smagorinsky closure [18]. The SGS scalar flux is represented with a gradient law, $Q_{\alpha,j} = -\bar{\rho} \Gamma_{SGS} \partial \tilde{\phi}_\alpha / \partial x_j$, where $\tilde{\phi}_\alpha$ is the resolved scalar field and Γ_{SGS} denotes the subgrid diffusion coefficient evaluated from $\Gamma_{SGS} = \bar{\rho} (C_s \Delta)^2 |\tilde{S}| / Sc_{SGS}$ with Sc_{SGS} a subgrid scale turbulent Schmidt number.

The accurate determination of the filtered chemical reaction rate \bar{S}_α remains one of the most important challenges when applying LES to turbulent reactive flows. We retain herein a formulation that accounts for the subgrid scale fluctuations of the chemical composition through a modeled transport equation for the subgrid scale FDF, which provides an effective resolution to the closure problems that arise from averaging or filtering the highly nonlinear chemical source terms [2]. Since one-point one-time FDF models are used, the terms that involve two points information, i.e., some property gradients, are not explicitly resolved, hence important effects, such as molecular diffusion and viscous effects, and associated dissipation phenomena require to be modeled.

The modeled transport equation for the scalar PDF is written as:

$$\begin{aligned} & \frac{\partial}{\partial t} \rho(\Psi) P_\Phi(\Psi; \mathbf{x}, t) + \frac{\partial}{\partial x_j} \rho(\Psi) \tilde{u}_j P_\Phi(\Psi; \mathbf{x}, t) \\ & = \frac{\partial}{\partial x_j} \left[\rho(\Psi) (\Gamma + \Gamma_{SGS}) \frac{\partial P_\Phi(\Psi; \mathbf{x}, t)}{\partial x_j} \right] \\ & + \frac{\partial}{\partial \psi_\alpha} [\rho(\Psi) \Omega_m (\psi_\alpha - \langle \phi_\alpha \rangle) P_\Phi(\Psi; \mathbf{x}, t)] \\ & - \frac{\partial}{\partial \psi_\alpha} [S_\alpha(\Psi) P_\Phi(\Psi; \mathbf{x}, t)], \end{aligned} \quad (4)$$

where the chemical reaction term appears in closed form, thus circumventing the difficulties associated with the physical modeling of its filtered contribution. The derivation of such a transport equation may be found elsewhere [2]. The retained hypotheses are: (i) the conditional filtered velocity has been decomposed into filtered and subgrid contributions, with the latter closed by a turbulent diffusivity approximation, (ii) the conditional mixing term is closed by the IEM mixing model [19] also often referred to as the linear mean-square estimation (LMSE) model [20]. In the above equation,

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