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Stochastic modeling of atomizing spray in a complex swirl injector using large eddy simulation

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Abstract

Large-eddy simulation of an atomizing spray issuing from a gas-turbine injector is performed. The filtered Navier–Stokes equations with dynamic subgrid scale model are solved on unstructured grids to compute the swirling turbulent flow through complex passages of the injector. The collocated grid, incompressible flow algorithm on arbitrary shaped unstructured grids developed by Mahesh et al. (*J. Comp. Phys.* 197 (2004) 215–240) is used in this work. A Lagrangian point-particle formulation with a stochastic model for droplet breakup is used for the liquid phase. Following Kolmogorov's concept of viewing solid particle-breakup as a discrete random process, the droplet breakup is considered in the framework of uncorrelated breakup events, independent of the initial droplet size. The size and number density of the newly produced droplets is governed by the Fokker–Planck equation for the evolution of the *pdf* of droplet radii. The parameters of the model are obtained dynamically by relating them to the local Weber number and resolved scale turbulence properties. A hybrid particle-parcel is used to represent the large number of spray droplets. The predictive capability of the LES together with Lagrangian droplet dynamics models to capture the droplet dispersion characteristics, size distributions, and the spray evolution is examined in detail by comparing it with the spray patternation study for the gas-turbine injector. The present approach is computationally efficient and captures the global features of the fragmentary process of liquid atomization in complex configurations.

Keywords: Sprays; LES; Complex geometries; Droplet breakup; Stochastic models

1. Introduction

Liquid spray atomization plays a crucial role in analyzing the combustion dynamics in many propulsion related applications. This has led researchers to focus on modeling of droplet formation in numerical investigations of chemically reacting flows with sprays. In the traditional approach for spray computation, the Eulerian equations for gaseous phase are solved along with a Lagrangian model for droplet transport with two-way coupling of mass, momentum, and

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energy exchange between the two phases [1]. The standard approach is to first perform spray patternation studies for the injector used in combustion chambers and measure the size distributions at various cross-sections from the injector. These distributions are then used as an *input* to a numerical simulation which then computes the secondary atomization of the injected droplets. The secondary atomization is typically modeled by standard deterministic breakup models based on Taylor Analogy Breakup (TAB) [2], or wave [3] models. However, this requires performance of experimental tests for any new injector design which can be very costly.

Development of numerical approaches for direct simulations of the primary atomization of a liquid jet or sheet is necessary. However, such approaches also require significant computational effort. Such numerical schemes capture the complex interactions and instabilities near the gas–liquid interface, formation of ligaments and their disintegration into droplets. Considerable advances have been made in this area [4–6]. The predictive capability of such schemes may be strongly influenced by the grid resolutions used and capabilities for realistic injector geometries are still under development.

Majority of spray systems in propulsion applications involve complex geometries and highly unsteady, turbulent flows near the injector. The numerical models for spray calculations should be able to accurately represent droplet deformation, breakup, collision/coalescence, and dispersion due to turbulence. Simulations involving comprehensive modeling of these phenomena are rare. Engineering prediction of such flows relies predominantly on the Reynolds-averaged Navier–Stokes equations (RANS) [7,8]. However, the large-eddy simulation (LES) technique has been convincingly shown to be superior to RANS in accurately predicting turbulent mixing in simple [9], and realistic [10–12] combustor geometries. It was shown that LES captures the gas-phase flow physics accurately in swirling, separated flows commonly observed in propulsion systems. Recently, Apte et al. [13] have shown good predictive capability of LES in swirling, particle-laden coaxial combustors. The particle-dispersion characteristics were well captured by the Eulerian–Lagrangian formulation.

In this work, LES together with a stochastic subgrid model for droplet atomization is used for simulation of spray evolution in a real gas-turbine injector geometry. Modeling of the complexities of the atomization process is based on a stochastic approach. Here, the details of the ligament formation, liquid sheet/jet breakup in the near injector region are not computed in detail, but their global features are modeled in a statistical sense. Following Kolmogorov's concept of viewing solid particle-breakup as a discrete random process [14], atomization of liquid drops at high relative liquid-to-gas velocity is considered in the framework of uncorrelated breakup events, independent of the initial droplet size. Gorokhovski and Saveliev [15] reformulated Kolmogorov's discrete model of breakup in the form of a differential Fokker–Planck equation for the *pdf* of droplet radii. The probability to break each parent drop into a certain number of parts is assumed independent of the parent-drop size. Using central limit theorem, it was pointed out that such a general assumption leads to a log-normal distribution of particle size in the long-time limit. This approach was further extended in the context of large-eddy simulations of the gas-phase by Apte et al. [16] and validated for spray evolution in simplified diesel engine configuration.

In this work, the stochastic breakup model is applied to simulate a spray evolution from a realistic pressure-swirl injector to evaluate the predictive capability of the model together with the LES framework. As the first step, cold flow simulation with stochastic model for secondary atomization is performed. This study thus isolates the problem of liquid atomization in pressure-swirl injectors typically used in gas-turbine engines and serves as a systematic validation study for multiphysics, reacting flow simulations in realistic combustors [12].

In subsequent sections, the mathematical formulations for the large-eddy simulation of the gaseous-phase and subgrid modeling of the liquid phase are summarized. Next, the stochastic model for liquid drop atomization is discussed together with a hybrid particle-parcel algorithm, based on the original parcels approach proposed by O'Rourke and Bracco [17], for spray simulations. The numerical approach is then applied to compute unsteady, swirling flows in a complex injector geometry and the results are compared with available experimental data on spray patternation studies.

2. Mathematical formulation

The governing equations used for the gaseous and droplet phases are described briefly. The droplets are treated as point-sources and influence the gas-phase only through momentum-exchange terms [13].

2.1. Gas-phase equations

The three-dimensional, incompressible, filtered Navier–Stokes equations are solved on unstructured grids with arbitrary elements. These equations are written as

$$\frac{\partial \overline{u}_i}{\partial t} + \frac{\partial \overline{u}_i \overline{u}_j}{\partial x_j} = -\frac{\partial \phi}{\partial x_i} + \frac{1}{Re_{\text{ref}}} \frac{\partial^2 \overline{u}_i}{\partial x_j x_j} - \frac{\partial q_{ij}}{\partial x_j} + \overline{\dot{S}}_i, \qquad (1)$$