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Large-eddy simulation of shear flows and high-speed vaporizing liquid fuel sprays

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ABSTRACT

Large eddy simulation models are tested for use on high speed evaporating liquid sprays. Three models are tested: standard Smagorinsky, a one-equation viscosity based model, and the dynamic structure model. The models are tested using channel flow, planar gas jet, and a diesel spray. The motivation of the work is to evaluate the accuracy and suitability of LES models that can be used for internal combustion engine modeling with direct injection of fuel in which moderate mesh resolution is the norm. Results from the channel flow and the gas jet provide additional insight into model capabilities that impact performance in liquid spray simulations. Simulation results were analyzed using contour images to compare the general structure of the flows, and experimental data for comparison of ensemble averaged mean and rms velocity profiles, liquid and vapor penetration, and mass fraction profiles. Results show that all three models perform similarly in the channel flow with good matches on the mean velocity results and some under prediction of rms values. The dynamic structure model showed slightly steeper near wall rms values closer to the experimental data. In the jet flow, the one-equation model results showed unexpected flow structures in images of the velocity magnitude. Mean velocity profiles matched data well for all three models. But centerline velocity decay rates and rms velocity radial profiles matched data much better for the dynamic structure model results. In the liquid spray the one-equation model performed poorly when compared to experimental data. The Smagorinsky model gave reasonable results and the dynamic structure model gave very good results in these comparisons. The overall conclusion is that the dynamic structure model is the best of the three models for direct injection engine simulations.

1. Introduction

In computational fluid dynamics simulations turbulence modeling is often a key component for achieving accurate predictions. Large eddy simulation (LES) turbulence modeling has become more prevalent and can offer advantages over traditional Reynolds averaged Navier Stokes (RANS) modeling. Commonly used LES subgrid models are reviewed by Meneveau and Katz [1] and Piomelli [2]. Sub-grid models for LES have been well developed and are widely tested in many simple incompressible flows, such as homogeneous and isotropic turbulence and channel flows. More recently LES is being used to simulate more complex flows in real engineering applications including chemically reacting flows, highly compressible flows, and multiphase flows (e.g., Refs. [3–5]).

In this study, we are particularly interested in using LES to model high-speed liquid fuel sprays, especially sprays that are found in internal combustion (IC) engines. Due to the high injection pressure difference (on the order of 10^1–10^2 MPa) and the small nozzle hole (on the order of 10^2 μm), the liquid fuel atomizes, vaporizes, and finally combusts. This process greatly impacts the efficiency and emissions of IC engines. It is highly unsteady, three-dimensional, and thus the conventional ensemble-averaged method such as Reynolds-averaged Navier–Stokes (RANS) can easily miss some of the important temporal and spatial fuel–air mixing details that are important for accurate predictions. On the other hand, LES can be more appropriate since it can predict more flow structures than RANS and these flow structures, eddies, and vortices affect and are affected by the liquid spray. Turbulence and flow structures in a direct injection combustion chamber are generated by high shear arising from the high-speed liquid fuel. In practical engineering LES of high-speed fuel sprays, fine mesh resolution, which is capable of resolving the shear layer near the injector region, is usually not desirable due to the computational cost. Thus, an LES model that works well on a relatively coarse mesh resolution is required. In addition, several issues regarding LES of sprays were pointed out by Rutland [6], who reviewed the fundamental work done by Bellan et al. [7–11] One of these issues

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is that a good LES model is required to correctly capture the large scale and the sub-grid interaction with liquid droplets. LES spray modeling is challenging and there are few studies evaluating LES models in high-speed liquid fuel sprays in the context of engineering LES. Thus, the main purpose of this paper is to test several commonly used LES models in this type of flows.

Constant volume spray bombs are good test cases for studying LES of sprays due to their simple geometry and abundant experimental data such as that from the Engine Combustion Network (ECN) [12]. Hori et al. [13] used the one-equation eddy-viscosity sub-grid model [14,15] accompanied by spray models mainly developed for RANS to simulate a spray bomb and found that spray penetrations are strongly dependent on mesh resolution. Satisfactory spray tip penetration comparisons were obtained when the grid size (0.12 mm) was smaller than the diameter of the nozzle hole (0.2 mm). However, this grid size is not practical for engineering applications. The mesh resolution used in our study is much lower than the study of Hori et al. Although various approaches are adapted in engineering simulations of sprays such as the gas jet model [16], none of these are used in this study since some LES model effects may be hidden behind these remedies.

Before testing the performance of models on sprays, the LES models are evaluated on "building -block" flows [2]. These flows have simple geometry and at least one homogeneous direction. In this study, fully-developed channel flow and planar gas jet were chosen as building block flows to test LES models. Both of these flows generate turbulence and flow structures through a dominate shear mechanism similar to high-speed liquid fuel sprays. In addition, the planar gas jet configuration is analogous to the liquid fuel sprays even though the nozzle shapes are different and the planar gas jet is single-phase. Several studies have been done in testing LES models through the channel flow and the planar gas jet. For instance, Fureby et al. [17] evaluated the performance of eight different LES models in channel flow of three different Reynolds numbers with a fixed grid resolution. They found that larger scatter in the LES data could be observed as the Reynolds number increases. This indicates that the demands on the LES models increases as the Reynolds number increases. Le Ribault et al. [18] used the standard Smagorinsky model [19], the dynamic Smagorinsky model [20] and the dynamic mixed model [21] to simulate a planar gas jet with Reynolds numbers of 3000 and 30,000 and found that, in general, models deriving from the dynamic procedure [20] could predict turbulent intensities better. Liu et al. [22] did similar studies for the planar gas jet with a Reynolds number of 4000 with five different LES models. However, these two studies compared flow statistics only in a region less than $x/d = 20$, and focused mostly on relatively low Reynolds number cases (3000 and 4000) which are not typical for engineering applications. In this study, flow statistic properties in the region of $x/d > 40$ and the Reynolds number of 30,000 are studied.

In this paper, three LES models are used in simulating channel flow, a planar gas jet and a high-speed diesel liquid fuel spray in a constant volume chamber. Results are compared against available experimental and direct numerical simulation (DNS) data. The three LES models are the standard Smagorinsky model [19], the one-equation eddy viscosity model [14,15], and the dynamic structure model [23]. The first two models are viscosity-based with constant model coefficients and are widely used in fundamental studies as well as engineering applications (e.g., Refs. [24,25]). Thus, it is of interest to see the suitability of these two simple and robust models applied in liquid spray simulations. The non-viscosity dynamic structure model [23] has been widely used in many internal combustion engine simulations [26–28], and acceptable results such as pressure traces and heat release rates can be obtained. In this paper, we have modified the original dynamic structure model by including an additional artificial viscosity term in the near nozzle region to accommodate the high strain rates which usually occur in diesel sprays. Details and validations of this model are discussed in subsequent sections. All of the simulations are performed using OpenFOAM version 2.1.1 [29].

The first part of this paper describes the governing equations and the three LES sub-grid models. The second part, the third part and the fourth part show numerical setups and results of the channel flow, the plane gas jet and the vaporizing spray in a constant volume chamber, respectively. Differences between the results predicted by the three LES models and the experimental or the DNS results are discussed. The paper closes with a summary and conclusions.

2. Governing equations

In LES, any flow variable $F(\boldsymbol{x}, t)$ can be decomposed as

$$F(\boldsymbol{x}, t) = \overline{F}(\boldsymbol{x}, t) + F'(\boldsymbol{x}, t) \tag{1}$$

where

$$\overline{F}(\boldsymbol{x}, t) = \int G(\boldsymbol{r}, \boldsymbol{x}) F(\boldsymbol{x} - \boldsymbol{r}, t) d\boldsymbol{r}, \tag{2}$$

and G is a low-pass filter function depending on the filter length Δ and $F'(\boldsymbol{x}, t)$ is the sub-grid variable. Common filter functions are box and Gaussian functions. For the compressible Navier–Stokes equations, the Favre averaging is frequently used. It is defined as $\widetilde{F}(\boldsymbol{x}, t) = \overline{\rho F(\boldsymbol{x}, t)}/\bar{\rho}$ where ρ is the fluid density.

Applying the filtering operation to the Navier–Stokes equations leads to the following governing equations [30].

<u>Filtered continuity equation</u>

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j}{\partial x_j} = \bar{\dot{S}}_{mass} \tag{3}$$

<u>Filtered momentum equation</u>

$$\frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i \tilde{u}_j}{\partial x_j} = -\frac{\partial \overline{P}}{\partial x_i} + \frac{\partial \bar{\tau}_{ij}}{\partial x_j} - \frac{\partial \bar{\rho} \Gamma_{ij}}{\partial x_j} + \bar{\dot{S}}_{momentum} \tag{4}$$

<u>Filtered energy equation</u>

$$\frac{\partial \bar{\rho} \tilde{h}_t}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j \tilde{h}_t}{\partial x_j} = \frac{\partial \overline{P}}{\partial t} - \frac{\partial \bar{q}_j}{\partial x_j} - \frac{\partial h_j^{sgs}}{\partial x_j} + \bar{\dot{S}}_{energy} \tag{5}$$

<u>Filtered species transport equation</u>

$$\frac{\partial \bar{\rho} \widetilde{Y}_l}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j \widetilde{Y}_l}{\partial x_j} = \frac{\partial \overline{\Phi}_{j,l}}{\partial x_j} - \frac{\partial \Phi_{j,l}^{sgs}}{\partial x_j} + \bar{\dot{S}}_{species,l(l=1,\ldots,N-1)} \tag{6}$$

where N is the total number of chemical species. The source terms $\bar{\dot{S}}_{mass}$, $\bar{\dot{S}}_{momentum}$, $\bar{\dot{S}}_{energy}$, and $\bar{\dot{S}}_{species,l}$ correspond to the interaction of the gas flow field with the spray and are described later in this section. The velocity field, thermodynamic pressure, and mass fraction for species l are denoted respectively by u, P, and Y_l. The total specific enthalpy, h_t, is defined as $\int_{T_0}^{T} C_{Pd} T' + 1/2 u_k u_k$, where T is the temperature, T_0 is the reference temperature (298.15 [K]) and C_P is the specific heat at constant pressure. The pressure and the temperature can be related using the ideal gas equation, $\overline{P} = \bar{\rho} R \widetilde{T}$. The filtered viscous stress tensor, $\bar{\tau}_{ij}$, filtered heat flux, $\bar{q}_j$, and filtered species flux, $\overline{\Phi}_{j,l}$ are given respectively by

$$\bar{\tau}_{ij} = \overline{\rho \nu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right)} \approx \bar{\rho} \nu \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} - \frac{2}{3} \frac{\partial \tilde{u}_k}{\partial x_k} \delta_{ij} \right) \tag{7}$$

$$\bar{q}_j = \overline{-\alpha \rho C_P \frac{\partial T}{\partial x_j}} \approx -\alpha \bar{\rho} C_P \frac{\partial \widetilde{T}}{\partial x_j}, \tag{8}$$

and

$$\overline{\Phi}_{j,l} = \overline{\rho D_l \frac{\partial Y_l}{\partial x_j}} \approx \bar{\rho} D_l \frac{\partial \widetilde{Y}_l}{\partial x_j}, \tag{9}$$