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Numerical study of high speed evaporating sprays

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ABSTRACT

Large eddy simulations of high speed evaporating sprays are conducted to study spray interactions with the gas flow and turbulence generated by the spray. The spray is simulated with a Lagrangian droplet method and a stochastic breakup model together with non-equilibrium, finite-rate heat and mass transfer models. The Lagrangian spray/droplet field is fully coupled with the Eulerian gas flow through mass, momentum and energy coupling terms. The interaction of spray induced gas flow and turbulence with the droplets is studied for different gas chamber densities and temperatures as well as different nozzle sizes and injection pressures. Our results indicate that although the droplet transport and evaporation are both important to the generated gas flow and its interactions with the spray, the major source of momentum transfer to the gas is the high speed vapor generated by evaporation. It is shown that sprays injected from larger nozzles generate more perturbations in the gas due to increase in evaporation rate by higher entrained gas. However, the liquid spray penetration remains unchanged with the variation in injection pressure due to competing effects of evaporation and vapor convection. While the liquid penetration is not significantly affected by the injection pressure, the evaporated vapor penetrates more and mixes better at higher injection pressures due to higher induced gas velocity and turbulence.

Introduction

High speed evaporating sprays and their two-way mass, momentum and energy interactions with the gas flow turbulence are important in advanced combustion systems. The mass and volume of the dispersed liquid with respect to the carrier gas are two of the critical parameters that determine the level of interaction between phases. Flows containing very small (in comparison to the Kolmogorov scale) droplets with small mass and volume fraction have gas flow and turbulence structure similar to that of a single-phase flow. However, with larger droplets and higher volume fractions, the liquid effects on gas turbulence production, dissipation and stresses become important (Crowe et al., 1998; Sirignano, 2010; Balachandar and Eaton, 2010). This, of course, depends on the spray speed and the level of background gas turbulence. When a spray is injected with low to moderate speeds into a quiescent chamber, the gas flow and turbulence stay insignificant. However, at high injection pressures and for high speed sprays (order of hundreds of meter per second), spray droplets can become a significant source of gas turbulence. This is partly due to drag of liquid droplets but can also be caused by the droplet evaporation as shown below. Balachandar and Eaton (2010) considered the main mechanisms for flow/turbulence modifications by non-evaporating droplets to be: (i) the drag of larger droplets causing enhanced dissipation, (ii) the transfer of droplet kinetic energy to the gas, (iii) the wakes and vortex shedding behind large droplets and (iv) the buoyancy induced instabilities due to density variations arising from the preferential concentration of droplets. Depending on the ratio of the dispersed phase response time to the flow time scale, known as the Stokes number, *St*, the dispersed phase particles change both the dissipation and the production of carrier fluid turbulence. For sprays issuing into a quiescent chamber with high injection pressures, the generated droplets have high velocities and large *St* numbers. Consequently, the droplet wake and enhanced dissipation mechanisms play lesser roles and the turbulence is mainly generated and modified by the droplet drag and the evaporation as explained below.

Two general types of computational models have been developed for numerical simulations of two-phase flows involving sprays (Balachandar and Eaton, 2010; Prosperetti and Tryggvason, 2007; Subramaniam, 2013). In the Eulerian–Lagrangian models, the continuous carrier phase is described by the Navier–Stokes equations on Eulerian grid points, while the spray is represented by discrete droplets, which are injected and tracked in the computational domain in a Lagrangian manner. The two-fluid Eulerian–Eulerian models treat the carrier fluid and the dispersed phase as "interpenetrating media" which are described by a set of mass, momentum and energy conservation equations. The Eulerian–Eulerian models assume the existence of unique field

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representations for particle velocity and temperature, implicitly restricting the maximum *St* number that can be considered (Balachandar and Eaton, 2010). The primary jet breakup in sprays can be simulated by Eulerian–Eulerian models (Gorokhovski and Herrmann, 2008; Shen and Yue, 2001; Li and Jaberi, 2009; Herrmann, 2010). These types of models are expected to better capture the main liquid jet breakup, but they are not currently practical and cannot be employed for high speed evaporating sprays in realistic systems. Far enough from the injector nozzle, the liquid droplets are small, dispersed and far from being a continuum. Consequently, they can be better represented by a collection of Lagrangian particles.

The method we refer to as the direct numerical simulation (DNS) can accurately capture the two-way interactions of particles with the carrier turbulent flow. However, DNS is extremely demanding and currently impractical for high speed turbulent sprays. Large eddy simulation (LES) method on the other hand has been widely applied to multiphase flows and can be a viable tool for spray simulations (Fox, 2012), even though submodels are required in LES to account for various physical processes taking place at small or subgrid time and length scales in both Eulerian and Lagrangian fields. LES models have been recently applied to complex systems involving evaporating/reacting sprays and complex droplet-turbulence interactions at resolved and subgrid scale (SGS) levels (Moin and Apte, 2006; Patel and Menon, 2008; Banaeizadeh et al., 2013; Bini and Jones, 2009; Bharadwaj et al., 2009; Irannejad and Jaberi, 2014; Irannejad et al., in press). A number of spray LES studies have been focused on flows in complicated geometries (Moin and Apte, 2006; Patel and Menon, 2008; Banaeizadeh et al., 2013), while others discussed various SGS modeling issues. Bini and Jones (2009) indicated the importance of SGS models for evaporating sprays. It was pointed out that the neglect of SGS acceleration and vaporization of droplets causes poor predictions of the spray and the carrier fluid flow. Patel and Menon (2008) and Bharadwaj et al. (2009) included the subgrid spray drag force fluctuations in the SGS kinetic energy equation. Irannejad and Jaberi (2014) included the added mass contribution to the carrier gas kinetic energy at the subgrid level in their LES study. They also considered other physical phenomena that affect the spray behavior such as the modification of droplet dynamics by wake interactions and the transient heating of droplets' interior. Following this work, we use a similar LES/spray model in the present paper to study the physical behavior of turbulent flows generated by high speed evaporating sprays and the interactions that these flows have with the droplets under variety of flow and spray operating conditions.

Turbulence interactions with dispersed particles or droplets have been extensively studied in the past (Balachandar and Eaton, 2010; Hetsroni, 1989; Elghobashi and Truesdell, 1993; Mashayek and Pandya, 2003). Most of these studies were on the modulation of turbulence by particles (Crowe, 2000; Eaton, 2006; Eaton, 2009). However, some studies also considered the turbulence generation by the dispersed phase (Chen et al., 2000). Earlier numerical studies were focused on the isothermal and non-evaporating particle-laden flows. In flows with evaporating particles, additional complexities due to combined effects of interphase heat and mass transfers and turbulent mixing of particle vapor arise. Birouk and Gokalp (2006) reviewed studies conducted on the effect of turbulence on individual droplets. Most of these studies show that with increasing the turbulence level, the evaporation rate is increased. However, in an evaporating spray, droplets can significantly change the vapor mass fraction and other flow variables around droplets, which can in turn change the droplet evaporation. Reveillon and Demoulin (2007) in their DNS study, investigated the one way interaction of a forced isotropic turbulent flow with evaporating droplets at different Stokes numbers ($St = 0.17$, 1.05 and 5.6) and found very different behavior. It was shown that droplet clusters are created because of the turbulence, leading to local vapor concentration and in turn slowing down of the droplet vaporization rate. The standard deviations of vapor concentration fluctuations, which were mostly attributed to the presence of droplet clusters, were strongly dependent on the Stokes number. On the other hand, there have been several studies on the two-way interactions of evaporating droplets with the gas turbulence. DNS and LES studies (Mashayek, 1998; Miller and Bellan, 1999; Okongo and Bellan, 2004; Leboissetier et al., 2005) of droplet-laden homogeneous shear and temporal shear layer flows, for example, showed that the droplet evaporation increases the turbulent kinetic energy and the dissipation of turbulent kinetic energy of the carrier gas. Understandably, the majority of previous DNS and LES studies were focused on mono-dispersed droplets with low to moderate droplet Stokes numbers ($St \leq 1$). Experimental studies indicate that poly-dispersity of droplets can cause significant fluctuations in vapor concentration in highly turbulent flows (Cochet et al., 2009). Presently, our understanding of high speed poly-dispersed evaporating sprays is somewhat limited due to droplet poly-dispersity, interphase heat and mass transfers and complex interactions of high Stokes number ($St \gg 1$) droplets with the gas flow and turbulence.

This paper is on the detailed study of gas flow mass, momentum and energy interactions with very high speed evaporating droplets in sprays. The focus is on the flow and turbulence generated by the spray in the gas and the effects that they have on the spray/droplet evolution. Details of the computational model and the sensitivity of numerical results to various spray and LES submodels are discussed in our previous paper (Irannejad and Jaberi, 2014). The intent here in this paper is to better understand the complicated processes involved in high pressure sprays injected in high temperature and pressure chambers. Our results below show the importance and the complexity of the flow and turbulence generated by the spray.

Mathematical formulation and numerical solution

The two-phase LES model used in this work has two main mathematical components: (1) the Eulerian gas conservation equations, and (2) the Lagrangian spray equations. Fig. 1 shows various submodels embodied in the two components of LES/spray solver. As shown in this figure, for the carrier gas velocity, pressure and scalars we solve standard (Eulerian) filtered equations with appropriate SGS models. The spatial discretization of the carrier gas equations is based on the fourth-order compact finite difference scheme and the time differencing is based on a third order low storage Runge–Kutta method (Banaeizadeh et al., 2013; Irannejad and Jaberi, 2014; Afshari et al., 2008). The subgrid turbulence is modeled by a SGS kinetic energy equation that includes the spray effects on the SGS turbulence. The spray is simulated with a non-equilibrium Lagrangian particle method. The effect of SGS turbulence on the droplet is included through a stochastic subgrid model. The modification of droplet dynamics by wakes of nearby droplets is also considered. The spray breakup is modeled by a stochastic equation for the droplet size distribution. Heat and mass transfers between phases are calculated by solving mass and energy conservation equations for the droplet interior and surface. The Lagrangian spray equations are fully coupled with the Eulerian gas equations through mass, momentum, energy and species source/sink terms. The two components of the LES/spray model are further described in the following sections. More details can be found in Ref. (Irannejad and Jaberi, 2014).

Eulerian filtered gas equations

The gas phase compressible Favre-filtered continuity, momentum, energy and species mass fraction (scalar) equations are