High Fidelity Simulations of Turbulent Spray Combustion

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Abstract—A high–fidelity two-phase large eddy simulation (LES)/filtered mass density function (FMDF) model is developed and used for detailed simulations of turbulent spray breakup, evaporation and combustion. The spray is simulated with Lagrangian droplet transport, stochastic breakup, wake, collision/coalescence and finite rate heat and mass transfer submodels. The spray model is used together with the compressible, Eulerian LES gas flow model for velocity and pressure fields and the two-phase Lagrangian FMDF for the scalar (species mass fraction and enthalpy) field. There are two-way couplings between all Lagrangian and Eulerian models. The numerical results for non-reacting and reacting sprays are compared with the available experimental data for global spray variables such as the spray penetration length, ignition delay and flame lift-off lengths. It is shown that the two-phase LES/FMDF results are consistent and compare well with the experimental data.

Keywords: Turbulent Sprays, Liquid Spray Flames, LES of Reacting Sprays, Two-phase FMDF

I. INTRODUCTION

Liquid fuel sprays are important to advanced combustion and propulsion systems. The spray interactions with the flow and combustion in these systems are complex and are dependent on a significant number of parameters like the fuel supply operating pressure and temperature, the nozzle geometry, the physical and chemical properties of the liquid or droplets, the flow turbulence and all parameters controlling the heat and mass transfer between phases. Accurate prediction of the spray combustion often requires high fidelity models for the transport, breakup, evaporation and chemical reaction of liquid droplets in a turbulent environment. The challenge is to develop affordable models which can properly describe the complicated multiscale interactions among spray, turbulence and combustion.

One of the goals of spray simulation is the prediction of droplet size distribution and its evolution which is dependent on the spray/droplet breakup models. Kelvin-Helmholtz, Rayleigh-Taylor instability (KH-RT) [1] and Taylor analogy breakup (TAB) models [2] are considered as standard models for the spray breakup [3-4]. Recently, stochastic breakup models have gained some popularity, due to their ability to predict the (essential) global features of sprays without being computationally too expensive [5-10]. In these models, the distribution of droplet radii after the breakup is assumed to be a stochastic solution of a Fokker-Planck equation. Following this approach, the breakup frequency is computed here by a breakup velocity that is based on the Lagrangian gas to droplet relative velocity fluctuations. The fragmentation intensity spectrum is assumed to be Gaussian in accordance to Kolmogorov theory of discrete particle breakup [9-10].

In the denser regions of the spray, where the droplet number density is very significant, droplets start to modify the flow around them to such an extent that droplet behavior is also affected. While collision/coalescence can have a secondary effect on single hole sprays, droplet wake interaction can still be significant. Droplet-wake interactions are neglected in the majority of previous works on multi-dimensional spray simulations. In the present work, the aerodynamic wake effect of leading droplets on the relative velocity of the trailing droplets is implemented by the modification of relative velocity via correction functions which are based on the Reynolds number, droplet diameters, their positions and the direction of movement of droplets with respect to each other [9-10].

In most evaporating spray simulations, the modeling approach to evaporation has been that of assuming the inner droplet variables to be uniform [11]. Clearly, the presence of components with a wide range of volatility and the consequent non-monotonicity of species mass fractions and temperature fields inside fuel droplets demand more complex finite rate, multicomponent heat and mass transfer representation for the droplet [12-13] even though an assumption of spherical symmetry is usually necessary. Following Refs. [14-15], spherically symmetric heat and mass equations inside droplets are solved here together with droplet-gas interface equations for each individual droplet.

The conventional approach to the spray simulation is to solve the gas-phase equations by a grid-based Eulerian method and to compute the spray by a particle-based Lagrangian method [3,13,16]. In this approach, submodels are required to account for the various physical processes taking place at
“small” time and length scales in both Eulerian and Lagrangian fields. An important issue is the accurate modeling of gas flow interactions with the spray or droplets. For the gas flow simulations, spray models often rely predominantly on the Reynolds-averaged Navier-Stokes (RANS) method [3]. However, because of unsteady and turbulent nature of the gas flow generated by high speed sprays and other inherently transient physical and chemical processes involved in a typical spray combustion system, LES is expected to be more suitable than RANS [17]. Even with the hydrodynamic interaction of spray with the carrier gas is correctly simulated, the accuracy of spray simulations is still dependent on the models used for micro-mixing and highly nonlinear chemical reactions. Transported probability density function (PDF) methods have proven to be particularly effective in accounting for turbulence-chemistry interactions [18-19]. Filtered mass density function (FMDF) is a promising transported PDF method for LES of turbulent reacting flows which was developed based on the solution of single-point, subgrid-scale PDF of turbulent variables [20]. In this approach, the joint statistics of turbulent variables at subgrid level are obtained by solving the FMDF transport equation. The main advantage of FMDF is that the reaction terms appear in a closed form in its formulation. This allows simulations of various types of reactions (slow, fast, premixed, non-premixed, etc.) with complex chemical kinetic models [21-27]. Recently, the FMDF is extended to multiphase flows [26]. The two-phase LES/FMDF model is capable of capturing complex interactions among turbulence, combustion, and spray and has already been applied to various turbulent flames in conjunction with multi-step, non-equilibrium reaction models [25-27]. We apply the FMDF to high speed evaporating and reacting sprays in this paper.

II. MATHEMATICAL FORMULATION AND MODELING

The two phase LES/FMDF model consists of three major mathematical/computational components: (A) the Eulerian filtered gas dynamic equations, (B) the FMDF and its equivalent Lagrangian stochastic equations, and (C) the Lagrangian spray/droplet equations. There are two-way couplings among all Eulerian and Lagrangian fields.

A. Filtered Gas Dynamics

In this paper, the filtered compressible gas continuity, momentum, and energy equations are solved on Eulerian finite difference (FD) grid points for the velocity and pressure fields [10, 23, 25] with high-order compact finite difference and multi-step Runge-Kutta methods. The subgrid stresses and fluxes are modeled based on gradient type closures. The eddy viscosity is calculated from a two-phase subgrid kinetic energy model [10]. The subgrid kinetic energy is obtained by solving its transport equation with a high-order finite difference method.

B. Two-phase FMDF

The scalar field, i.e. reactive species mass fractions and enthalpy, is computed by solving the two-phase scalar FMDF equation. The FMDF transport equation is obtained by inserting the instantaneous unfiltered scalar equation into the time derivative of the fine grained density and spatial filtering [20]. For a compressible two-phase reacting system with small liquid volume fractions, the FMDF equation can be written in the following form [25-27]:

\[
\frac{\partial f_i^L}{\partial t} + \frac{\partial}{\partial x_j} \left( \frac{\partial}{\partial x_j} f_i^L \right) = \frac{1}{\rho} \frac{\partial}{\partial x_j} \left( \rho \frac{\partial}{\partial x_j} \psi \right) + \frac{1}{\rho} \frac{\partial}{\partial x_j} \left( \rho \frac{\partial}{\partial x_j} \psi \right) + \frac{1}{\rho} \frac{\partial}{\partial x_j} \left( \rho \frac{\partial}{\partial x_j} \psi \right) + \frac{1}{\rho} \frac{\partial}{\partial x_j} \left( \rho \frac{\partial}{\partial x_j} \psi \right) + \frac{1}{\rho} \frac{\partial}{\partial x_j} \left( \rho \frac{\partial}{\partial x_j} \psi \right)
\]

The first term in the right hand side (RHS) of Eq. (1) represents the SGS convection which is modeled with a gradient type closure. The term due to molecular diffusion (second term on the RHS of Eq. (1)) is decomposed into two parts, the molecular transport part and the SGS dissipation part. The SGS dissipation is modeled with the linear mean-square estimation (LMSE) or the interaction by exchange with the mean (IEM) model. The compressible source term due to pressure variation in the scalar FMDF is obtained by taking into account the total derivative of filtered pressure [28]. The last three terms in Eq. (1) represent the spray/droplet effects on FMDF. They involve particle source/sink terms affecting the gas composition and density. It is noted here again that in the FMDF equation, the highly non-linear complex reaction term (third term on RHS of Eq. (1)) is closed but in conventional LES methods it is not closed and has to be modeled.

The most convenient means of solving the FMDF transport equation is via the Lagrangian Monte Carlo (MC) procedure [29]. With the Lagrangian procedure, the FMDF is represented by an ensemble of computational “stochastic elements” (or “Monte Carlo particles”). These notional particles evolve via a stochastic process, described by a set of stochastic differential equations (SDEs). In the solution procedure, each MC particle is transported in the “physical space” by the combined actions of large scale convection and diffusion (molecular and subgrid). In addition, transport in the “composition space” occurs due to SGS/molecular mixing, chemical reaction, pressure variation and droplet heat and mass transfer [20, 26, 28]. To manage the number of MC particles and to reduce the computational cost, a procedure involving the use of non-uniform weights is considered [20]. The variable weighting for MC particles allows the particle number density to stay above a certain minimum value regardless of density variations. For the spray simulation, particle weights are modified due to added mass to the carrier gas by the evaporating droplets [26].

C. Lagrangian Droplets

The spray model considered in this chapter is based on the Lagrangian droplet method in which the droplet motion is computed via Basset Boussinesq Oseen (BBO) equation [13, 16]. The Basset force, the added mass term and the Saffman lift force are neglected in this equation. The gas velocity at droplet location is reconstructed based on the filtered velocity and a stochastic subgrid velocity [30]. The drag force is modeled...
based on Stokes time and the drag factor. The drag factor includes the effects of “finite slip” and “evaporative blowing” Reynolds number [31]. The droplet wake effect is dependent on the relative position, angle and size of nearby droplets and is taken into account through correction factors to the relative velocity [9-10]. To consider the effect of droplet collision, the model proposed by Munnanur and Reitz [32] is used in some of our simulations. Four possible collision outcomes of bouncing, coalescence, reflexive separation and stretching separation are considered.

A stochastic breakup model capable of generating a broad range of droplet sizes at high Weber numbers is used for predicting the new droplet formation. In this model, the size distribution of droplets generated by the breakup is based on the solution of a Fokker Planck equation whose main parameters are breakup frequency and the first two moments of the fragmentation intensity spectrum [6]. The breakup frequency and consequently the evolution of droplet diameter are assumed to be controlled by the relative velocity fluctuations between the gas and liquid phases [9-10].

The spherically symmetric, one-dimensional, multi-component unsteady continuity, energy and species equations inside each individual droplet are solved together with the following liquid-gas interface equations for obtaining the droplet variables at each time step [14]. For a multi-component droplet, the mass flux of species \( \alpha \) at the droplet interface may be written as

\[
\dot{m}_a = \phi_{\alpha a} 2\pi \alpha \rho_{\alpha} D_{\alpha} S_{\alpha} \ln(1 + B_{M_{\alpha}}),
\]

where the Spalding mass transfer number relates the liquid and gas interface mass fractions to the free stream (with respect to droplet) mass fraction. For the heat and mass transfer between droplet and surrounding gas, the well known Ranz-Marshall correlations for the Sherwood and Nusselt numbers are used. To account for the surface blowing effect of the evaporated liquid, Sherwood and Nusselt numbers are modified based on the film model of Abramzon and Sirignano [33]. The surface regression rate is then found by summing the mass flow rates over all species. The interphase coupling effects are represented by the conservation of mass for species \( \alpha \) and energy at the droplet interface as

\[
2r_\alpha \rho_{\alpha} \left[ (v_i - \dot{r}) (\phi_{\alpha i} - \phi_{\alpha i}) + 2r_\alpha \rho_{\alpha} D_{\alpha} \frac{\partial \phi_{\alpha i}}{\partial r_i} \right] - \rho_{\alpha} D_{\alpha} S_{\alpha} \ln(1 + B_{M_{\alpha}}) = 0
\]

\[
2r_\alpha \sum_i L_{i \alpha} \rho_{i} \left[ (\dot{r}_{i} - v_i) \phi_{\alpha i} + D_{\alpha i} \frac{\partial \phi_{\alpha i}}{\partial r_i} \right] - 2r_\alpha \lambda_{\alpha} \frac{\partial T}{\partial r_i}
+ \lambda_{\alpha} N_{\alpha} \left( T_{\alpha i} - T \right) = 0
\]

The effects of droplets on the carrier gas are included via a series of source/sink terms in the gas conservation equations. These terms are evaluated by volumetric averaging and interpolation of the Lagrangian droplet quantities for all the conservation equations as well as the subgrid kinetic energy equation. The spray terms in the FMDF equation are weighted averaged over the FD grid points and interpolated to the MC particle locations.

### III. Results and Discussions

The two-phase LES/FMDF model is used for simulations of non-evaporating and evaporating sprays with and without combustion. These are discussed in the following sections.

#### A. Non-Evaporating Sprays

The classical non-evaporating spray experiment of Hiroyasu and Kadota [34] is first simulated for the overall assessment of droplet transport and breakup models. Global spray variables such as the spray penetration length and droplet Sauter mean diameter (SMD) are measured at varying chamber pressures. Since the chamber temperature is relatively low, we refer to this experiment as non-evaporating spray experiment.

![Figure 1. Spray penetration length, obtained from LES and experimental (Exp.) data, at two chamber pressures (P).](image)

Figure 1 shows the spray penetration lengths predicted by the LES model at different times as compared with the experimental results. Overall, the LES results are in good agreement with the measured data. However, the predictions seem to be better at later times. The early values of liquid penetration are dependent on details of the liquid jet breakup near the nozzle which is modeled here by the breakup of big injected “blobs.” The model is not expected to be fully accurate in the flow region; however it can capture the droplet behavior further away from the nozzle and the longer time trends. The penetration length decreases with an increase in gas pressure as observed in Figure 1. At higher chamber pressures, the droplet breakup rate is higher and the numerical penetration values approach to the experimental values in a shorter time.

Figure 2 shows the droplet SMD at different axial locations as predicted by the present LES/spray model with and without collision and coalescence submodels, and by that of Apte et al. [7] for the chamber pressure of 1.1 MPa. Figure 2 also shows the experimental SMD, measured by Hiroyasu and Kadota at \( x=65 \text{mm} \) from the nozzle for the same spray. While the SMD values obtained by our LES model and that of Apte et. al. are similar without any collision/coalescence model, those obtained by our LES with the collision model show a slower decrease and a better comparison with the experiment at locations far from the nozzle, where the collision and coalescence are important in the absence of evaporation.
B. Evaporating Sprays without Combustion

The evaporating spray simulations are conducted for conditions close to those considered in experiments performed at Sandia National Laboratory as a part of engine combustion network (ECN) research [35-38]. In these experiments, the fuel spray behavior in a closed combustion chamber is studied.

Figure 3 shows the vorticity magnitude of the spray induced gas flow for the Sandia’s hexadecane spray, designated as spray CET. The three-dimensional (3D) vorticity contours in this figure clearly show the very significant and complex turbulent flow generated by the spray in the gas flow. The spray induced gas flow has a very significant effect on the dispersion, evaporation and mixing of the droplets and the evaporated fuel in the gas. Our results (not shown) indicate that more small scales are produced after main gas flow breakdown at higher chamber gas densities and temperatures.

Figure 3. Three-dimensional iso-level contours of the gas vorticity generated by the spray for $T=700$ K, $\rho=14.8$ kg/m$^3$.

For n-dodacane and n-heptane sprays, denoted as “Spray A” and “Spray H” by ECN, there are experimental data on transient liquid and vapor penetrations. The mean liquid penetration lengths are available for Spray CET, for a range of gas densities and temperatures as well as different nozzle sizes and injection pressures. Figure 4 shows the time variations of liquid fuel spray and vapor phase penetration lengths for Sprays A and H as obtained by the two-phase LES/FMDF model and compared with the experimental data. Figure 5 compares the experimental values of mean liquid penetration length with the simulated results for spray CET as a function of density for two different gas temperatures. The results in Figures 4 and 5 clearly show the capability of the two-phase LES/FMDF model to capture the global characteristics of the spray and the evaporated fuel in a highly unsteady and turbulent gas flow generated by the spray. Comparison of simulated and measured penetration lengths for different nozzle sizes and injection pressures (not shown) further confirms the reliability and accuracy of the spray LES model [17].

C. Evaporating Sprays with Combustion

The available experimental quantities for the reacting spray H are the ignition delay and the quasi-steady liftoff length [36, 38]. Variation of these global quantities with the ambient gas conditions is important and could be used for further
assessment of the global accuracy of the LES/FMDF/Spray model in comparison to experiments.

**Figure 6. Ignition delay at different gas temperatures.**

Figure 6 compares the simulated and measured ignition delay times at different ambient gas temperatures. LES/FMDF simulations are conducted with a 44 species skeletal mechanism for the chemical reaction [39]. The combustion chemistry calculation is accelerated via parallel in situ adaptive tabulation (ISAT) method [40-41]. It is to be noted that the ignition delay reported in the spray experiments considered in this paper comprises of a chemical delay and a physical delay. The physical delay deals with the spray breakup, evaporation and vapor mixing times and the chemical delay involves the generation of a radical pool and heat generating reactions. The physical delay analysis can be performed by non-reacting spray simulations conducted in previous section. The chemical delay depends both on the chemical kinetics model as well as the turbulence-chemistry interactions. Figure 6 shows that the numerical results are in good overall agreement with the experimental data. The comparison is very good at higher ambient (initial) gas temperatures. The simulated results, however, diverge from the experiment at lower initial gas temperatures. At lower temperatures, the flame ignition is a two stage process. The over-predicting trend of the simulated results is suggested to be mostly related to the chemical kinetic modeling [27].

**Figure 7. Flame visualization via OH radical mass fraction.**

Figure 7 shows the physical turbulent flame structure, visualized by the OH radical mass fraction, for the ambient gas temperature of $T=1000$ K. Clearly, the flame is lifted to a significant distance from the injector nozzle. Figure 8 compares the computed and experimental liftoff lengths as a function of gas temperature. For assessment of chemistry effect, the LES liftoff lengths are computed with a simple single-step global reaction model as well as the complex skeletal reaction mechanism. In contrast to ignition delay, which is sensitive to the chemical kinetics, the liftoff length is primarily dependent on the flow and turbulent chemistry interactions. This is supported by the observation that there is a good overall agreement between the LES/FMDF and experimental results.

**Figure 8. Comparison of measured spray flame liftoff lengths with simulated ones via different kinetics.**

Although the LES/FMDF conducted with the global reaction model perform rather poorly (the experimental and numerical ignition delays are very different and the computed liftoff lengths are shorter than the experiment), the trend in the liftoff length plots is similar and the numerical predictions become closer to the experiment at higher ambient gas temperatures even with this simple model. These results indicate that while the global reaction model is not quantitatively accurate, it is still useful for the overall study of the spray and testing of LES/FMDF/Spray submodels [42].

**IV. SUMMARY AND CONCLUSIONS**

The two-phase LES/FMDF model is used for numerical simulations of different non-evaporating and evaporating sprays with and without combustion. The LES/FMDF calculations are performed with a hybrid Eulerian-Lagrangian-Lagrangian mathematical/computational model. For the gas phase, the Eulerian Favre-filtered Navier-Stokes equations are solved together with subgrid turbulent kinetic energy equation. The scalar (species mass fraction and temperature) field is obtained by solving the two-phase FMDF equation with a Lagrangian MC particle method. The liquid spray simulation is also based on a Lagrangian model in which different submodels are employed for spray breakup, wake interactions, finite rate heat transfer and evaporation. Accuracy and reliability of the LES/FMDF/Spray model is assessed by comparing the model predictions with the experimental data for very different spray and flow conditions. For non-reacting sprays, the simulated liquid and vapor spray penetration lengths compare well with the experimental results despite strong turbulent gas flow generated by the spray. For reacting sprays, our results indicate that the flow and turbulence generated by the spray have a very significant effect on the flame structure. The ignition delays and flame liftoff lengths predicted by the LES/FMDF/Spray model with a skeletal reaction mechanism are shown to compare well with the experimental data.
ACKNOWLEDGMENT
This work was supported by the US Department of Energy under agreement DE-FC26-07NT43278. Additional support was provided by the Defense Logistics Agency under agreement DFARS-252232-7010. The authors wish to thank Professor Stephen Pope for providing the ISAT package. We would like to also acknowledge the computational resources provided by the HPCC at Michigan State University and the TACC supercomputing facility at UT-Austin.

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