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Large eddy simulation of a reacting spray flame with multiple realizations under compression ignition engine conditions

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ABSTRACT

An n-dodecane spray flame (Spray A from Engine Combustion Network) was simulated using a δ function combustion model along with a dynamic structure large eddy simulation (LES) model to evaluate its performance at engine-relevant conditions and to understand the transient behavior of this turbulent flame. The liquid spray was treated with a traditional Lagrangian method and the gas-phase reaction was modeled using a δ function combustion model. A 103-species skeletal mechanism was used for the n-dodecane chemical kinetic model. Significantly different flame structures and ignition processes are observed for the LES compared to those of Reynolds-averaged Navier–Stokes (RANS) predictions. The LES data suggests that the first ignition initiates in a lean mixture and propagates to a rich mixture, and the main ignition happens in the rich mixture, preferably less than 0.14 in mixture fraction space. LES was observed to have multiple ignition spots in the mixing layer simultaneously while the main ignition initiates in a clearly asymmetric fashion. The temporal flame development also indicates the flame stabilization mechanism is auto-ignition controlled. Soot predictions by LES present much better agreement with experiments compared to RANS, both qualitatively and quantitatively. Multiple realizations for LES were performed to understand the realization to realization variation and to establish best practices for ensemble-averaging diesel spray flames. The relevance index analysis suggests that an average of 5 and 6 realizations can reach 99% of similarity to the target average of 16 realizations on the mixture fraction and temperature fields, respectively. However, more realizations are necessary for the hydroxide (OH) and soot mass fractions due to their high fluctuations.

1. Introduction

Vehicles equipped with internal combustion engines (ICEs) will still be the main transportation tools in the foreseeable future. Due to their tremendous volume and high frequency of use, there are still immense benefits to obtain by continuously striving to increase the fuel efficiency and reduce emissions for these engines. In doing that, it is of paramount importance and, also extremely challenging, to understand the in-cylinder combustion process, e.g., cycle-to-cycle variations associated with the stochastic processes and varied ignition and emission characteristics due to local inhomogeneity [1]. In the last two decades, significant progress has been made in using experimental techniques to understand the in-cylinder process to assist engine design and optimization processes [2,3]. Despite these significant advancements, the state-of-the-art experiments can only provide partial information about the in-cylinder process due to the limitations of the measurement techniques. On the other hand, computational fluid dynamics (CFD) has been a critical complement in that context and can provide a complete, at least qualitative, picture of the in-cylinder process.

The Reynolds-averaged Navier–Stokes (RANS) turbulence model has been used extensively for diesel engine simulations due to its computational efficiency and it is expected to remain the mainstay turbulence model in the industry for the foreseeable future. Alternatively, large eddy simulations (LES) can potentially deal with complex flows by resolving a large disparity of length scales, which makes this turbulence model, although significantly more expensive, more attractive in the engine community. A detailed description of LES theory and modelling can be found in the literature by Pope [4,5] and a recent review of different LES turbulence models for engines can be found in the literature by Rutland [6].

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Recently, some LES studies have been performed in conjunction with different combustion models to examine its performance on diesel spray flame at engine-like conditions. Bekdemir et al. [7] implemented a flamelet generated manifold (FGM) model in the context of a Smagorinshky LES model and simulated a diesel spray flame. The mesh used had the minimum cell size of 0.08 mm near the nozzle exit and gradually increased to 0.8 mm in the downstream region, yielding about 4.3 million cells in total. The flame characteristics were well captured and it was demonstrated that the tabulation flamelet method could be used for LES engine simulations also. Tillou et al. [8] simulated a diesel jet using a Smagorinsky LES model coupled with a flamelet combustion model with tabulated chemistry and assessed the variability of spray combustion for 15 realizations. The mesh details were similar to the one in Ref. [7], but with 1.8 million total cells. It was concluded that the variability in terms of auto-ignition delay was negligible, with about a 10% variation on the heat release rate in the later stage of combustion. Ameen and Abraham [9] used a Smagorinsky LES model coupled with an unsteady flamelet progress variable (UFPV) model to simulate an n-heptane gas jet on a mesh with 7.9 million cells. The computational cells stretched from 0.05 to 0.1 mm axially (from nozzle exit to downstream region) and from 0.02 to 0.34 mm radially (from spray axis to the off-axis region). They analyzed the flame stabilization mechanism and compared the results to a RANS-based model. It was found that the ensemble-averaged quasi-steady lift-off length predicted by both LES and RANS were similar and the fundamental physics affecting the lift-off length were the same although the transient behavior was vastly different. Another LES study of a diesel reacting spray was conducted by Irannejad et al. [10], who used a LES-filtered mass density function (FMDF) method to assess the effect of turbulence-chemistry-interaction (TCI). The LES grid size was 0.2 mm in spray-axis direction and stretched on in other directions. There were 120 million Monte Carlo particles to statistically represent the flow field in the simulations. It was found that the main ignition first occurred in the fuel-rich regions and the flame lift-off was strongly dependent on the spray parameters, gas temperatures, and oxygen concentrations, etc. The most recent study is from Gong et al. [11] who investigated the auto-ignition and stabilization mechanisms of an n-dodecane spray flame at engine conditions using LES and detailed chemical kinetics models. A uniform mesh with cell size of 0.25 mm was adopted. It was found that two-stage ignition behavior was predicted, and auto-ignition and flame propagation were competing to explain the flame lift-off stabilization among the two ambient temperatures of 900 and 1000 K considered.

Progress has been made through those LES studies of reacting diesel flames. However, a systematic study of mesh resolutions, flame transient processes, multiple realizations, different ambient conditions, and soot predictions has been lacking. In this study, a δ function combustion model is used in conjunction with a dynamic structure LES model to simulate the Spray A condition associated with the Engine Combustion Network (ECN) [12]. The most significant difference of this study compared to the previous studies is that a systematic investigation is conducted on a high-fidelity resolution mesh with a cell size of 0.0625 mm in the entire spray and combustion regions. To the best of our knowledge, such fine mesh resolution is perhaps the most resolved LES study of the ECN spray flames and, in general, for the spray flames under compression ignition engine conditions. The high-fidelity data obtained are examined in detail in this paper and compared to those from a RANS-based model, and available experimental data. A similar LES study at coarser resolutions has also been performed in the past by Som et al. [13] and this study further extends the findings of Som et al.

The paper is organized as follows. The first part briefly describes the experimental data used to verify the modeling results, followed by a description of the model setup. The next section presents the studies of mesh resolution, detailed transient flame behaviors, "quasi-steady" state flame, different ambient temperature effect, soot predictions, and realization variations. The conclusion and summary are reported in the last section.

Table 1
Spray A experimental initial and boundary conditions.

Fuel	n-dodecane
Fuel temperature (K)	363
Nominal nozzle-hole diameter (μm)	90
Common-rail pressure (bar)	1500
Injection duration (ms)	6 (exp), 1.5 (sim)
Nozzle discharge coefficient	0.89
Ambient density (kg/m^3)	22.8
Ambient O_2 (%)	15[a]
Ambient temperature (K)	800–1200

[a] Mole fraction.

2. Experimental data

The spray experiments presented in this work were performed in a constant volume pre-burn chamber, which has provided a platform for model development and validation at engine relevant conditions [14–27]. A detailed description of the experimental setup and measurement procedures can be found in the literature [28–30]. Briefly, the combustion vessel is nearly cubical with an internal volume of approximately 1 L. Sapphire windows provide optical access to the spray event from four sides. Prior to and during operation, the temperature of the entire vessel is maintained at 461 K by electric heaters. Spark-ignition of a combustible gas mixture rapidly elevates the pressure and temperature within the vessel. The spray event (i.e., fuel injection) takes place when the desired thermodynamic conditions are achieved after a short cool-down period. These experiments used a common-rail diesel fuel injector equipped with a single 90-μm diameter orifice (#370) belonging to the family of Spray A ECN injectors. Some initial and boundary conditions are listed in Table 1.

Ignition delay times were measured using a high-speed camera operating at 20,000 frames/s. The camera was equipped with a 600-nm short pass filter to suppress the high-intensity soot luminosity, which permits collection over the camera's dynamic range. Quasi-steady lift-off lengths based on excited state OH (OH*) emission were measured by an intensified CCD camera equipped with a 308 nm (10 nm FWHM) bandpass filter. Time-resolved soot extinction images were obtained using a diffused, ultra-fast light-emitting diode (LED) setup with a second high-speed camera. The details of the extinction imaging experiment can be found in Manin et al. [31].

3. Computational setup

Fuel spray and combustion simulations were performed using the traditional Lagrangian-parcel Eulerian-fluid approach in the CFD software CONVERGE [32–34]. It incorporates models for spray injection, atomization and breakup, turbulence, droplet collision, and coalescence. The gas-phase flow field is described by using the Favre-averaged Navier–Stokes equations in conjunction with the LES-based turbulence models. The turbulence model includes source terms for the effects of dispersed phase on gas-phase turbulence. These equations are solved by using a finite volume solver. The details of these models can be found in a previous publication [35], so only a brief description is provided here.

3.1. Spray and combustion models

The dispersed phase is modeled using a traditional Lagrangian parcel method. The Kelvin–Helmholtz (KH) and Rayleigh–Taylor (RT) models are used to predict the droplet breakup [36,37]. Droplet collisions are modeled with no time counter (NTC) algorithm [38]. A