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Effects of Nozzle Diameter on Diesel Spray Flames: A numerical study using an Eulerian Stochastic Field Method

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Abstract

The present numerical study aims to assess the performance of an Eulerian Stochastic Field (ESF) model in simulating spray flames produced by three fuel injectors with different nozzle diameters of 100 μm , 180 μm and 363 μm . A comparison to the measurements shows that although the simulated ignition delay times are consistently overestimated, the relative differences remain below 28%. Furthermore, the change of the averaged pressure rise with respect to the variation of nozzle diameter is captured by the model. The simulated flame lift-off lengths also agree with the measurements, with a maximum relative difference of 13%. The spray flame produced by a larger nozzle diameter has a fuel-richer premixed core region despite the longer lift-off length, indicating that the higher fueling rate used with the larger nozzle diameter is a more dominating factor than the lift-off length is in influencing the air entrainment into the upstream of the spray flames. In addition, the simulated normalised flame lengths are found to decrease when the nozzle diameters increase. These predictions are in good qualitative agreement with the experimental observation. This work proves that the ESF model can serve as an important tool for the simulation of spray flames in marine diesel engines, where fuel injectors with different nozzle diameters are applied for pilot and main injections.

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Keywords: diesel spray flame; Eulerian Stochastic Fields; flame length; nozzle hole diameter; turbulent combustion

1. Introduction

With the mutual aim to reduce emissions from diesel engines, both automotive and maritime industries have been working on improving the understanding of in-cylinder processes, which is an important prerequisite to design

‘clean’ engines. To facilitate the study of diesel spray combustion, Sandia National Laboratory and numerous research groups share their optical measurements through the Engine Combustion Network (ECN) [1]. These measurements are used first, to improve the understanding of spray flame under high-pressure, high-temperature environment and second, for numerical model validation. In the case with reacting sprays, ignition delay time (IDT), flame lift-off length (LOL) and hydroxyl (OH) chemiluminescence measurements are usually used to evaluate the performance of turbulence-chemistry interaction (TCI) closure approaches. The commonly studied TCI closure approaches include Flamelet Generated Manifold, multiple Representative Interaction Flamelet, Conditional Moment-Closure and transported probability density function (PDF) [2]. Among all, the transported PDF model is one of the methods that has the capability to accurately simulate the auto-ignition phenomenon, the premixed mode and the diffusion flame with a single model [3,4]. The transported PDF model can be formulated in both the Lagrangian [1-3] and the Eulerian frameworks [4-6]. In the numerical studies where the Lagrangian-based transported PDF model was applied, the main focus has been to simulate spray flame structures at various ambient density, temperature and oxygen levels [1-3]. On the other hand, the Eulerian-based transported PDF model, which is also known as the Eulerian Stochastic Fields (ESF) model [5], has been gaining attention for the simulation of spray combustion under engine-like conditions [4,6]. Jangi et al. [4] implemented the ESF model to investigate the effects of fuel octane number on ignition and flame behaviors while Gong et al. [6] used it to study the diesel flame lift-off stabilisation in the presence of laser-ignition. In all these studies [1-5], the nozzle diameter is in the order of 100 μm , which is more relevant to light-duty automotive engine applications. The injector nozzle diameters in marine engines are generally larger in order to deliver a greater amount of fuel. For instance, the nozzle hole diameters in the medium-speed four-stroke marine engines simulated by Kyriakides et al. [7] and Kilpinen [8] were approximately four-fold larger at 370 μm and 388 μm respectively. More recently, Ishibashi and Tsuru [9] performed multiple injection experiments under marine engine-like conditions, in which the fuel injectors used to deliver pilot and main diesel fuel have different nozzle diameters of 160 μm and 500 μm respectively. The spray flame characteristics produced from each of these injections are expected to be different and have to be reproduced in order to provide an accurate prediction of the subsequent combustion and emissions formation processes. Set against these backgrounds, this work aims to validate the ESF model using experimental data obtained in an optical accessible constant volume chamber when three different nozzle diameters of 100 μm , 180 μm and 363 μm are used.

Nomenclature

CCM	Chemistry Coordinate Mapping
CFD	computational fluid dynamics
ESF	Eulerian Stochastic Field
IDT	ignition delay time
LOL	lift-off length
PDF	probability density function
TCI	turbulence-chemistry interaction
VPL	vapour penetration length

2. Numerical setup

The current multi-dimensional CFD spray combustion simulations are carried out using the open-source code, OpenFOAM version 3.0.1 [10]. A 90 degree sector domain is used to represent the constant volume chamber which has a cubic shape with side lengths of 108 mm. The injector is placed at the intersection of two cyclic boundaries. The isotropic cell size is set to 0.5 mm within the spray combustion region, which is found to reach mesh independence. The computational grid consists of approximately 89,000 cells. The time step size is fixed at 0.2 μs , which is found to reach stability without compromising the computational cost (not shown). The fuel spray, flow and combustion processes are modelled using the Eulerian-Lagrangian approach. The liquid properties of tetradecane are used to represent those of diesel fuel [11] while the Reitz-Diwakar model is used to simulate the fuel droplet breakup. The Realisable $k-\varepsilon$ model is employed for turbulence modelling due to its capability in predicting

the vapour penetration length (VPL) of the non-reacting diesel sprays (as shown later). The skeletal *n*-heptane model developed by Liu et al. [12] is used as the diesel surrogate model. The interaction between the turbulence and chemistry is simulated using the ESF method. In the current simulations, thirty-two stochastic fields are used and the mixing constant in the ESF model is fixed at two. The Chemistry Coordinate Mapping (CCM) method is coupled with the ESF solver in order to integrate the source terms due to chemical reactions efficiently [4,6]. The basic idea of the CCM method is to map the cells with similar thermochemical state in the physical space to several phase zones. It has been used in spray combustion modelling across a wide range of operating conditions [12]. Details about the ESF-CCM method can be found in reference [4]. Other CFD submodels used in the current simulations are similar to those reported by Gong et al. [6].

The operating conditions and injection specifications of the current test cases are listed in Table 1. The test case performed by Jangi et al. [4] is used as the reference case here. The ambient density and temperature are fixed at 14.8 kg/m^3 and 1000 K respectively, corresponding to an ambient pressure of approximately 40 bar . The fuel is delivered at an injection pressure of 1400 bar through an injector with a nozzle diameter of $100 \mu\text{m}$. Non-reacting spray data i.e. the liquid penetration length (LPL) and VPL are first used to validate the spray breakup, evaporation and turbulence model (case 1). Similar evaluation exercise is also performed for a larger nozzle diameter (case 2). The associated measurements are collected from different sources [1,13,14]. For all the reacting cases, the ambient oxygen concentration is set to 21% by mole fraction. The initial species mass fraction as well as flow and turbulence conditions can be found in the previous work [12]. The experimental IDT and LOL data are collected from the ECN database [1] and more descriptions on the reacting spray cases can be found in Refs. [15,16].

Table 1. Operating conditions and injection specifications in the current test cases.

Case	Ambient O ₂ level [%]	Ambient temperature [K]	Ambient density (kg/m ³)	Nozzle diameter (μm)	Injection pressure (bar)	Fuel mass flow rate (mg/ms)
1	0	1000	14.8	100	1400	2.7
2	0	1000	13.9	257	1400	14.0
3	21	1000	14.8	100	1400	2.7
4	21	1000	14.8	180	1400	8.8
5	21	1000	14.8	363	1400	35.8

3. Results and discussions

3.1. Non-reacting sprays

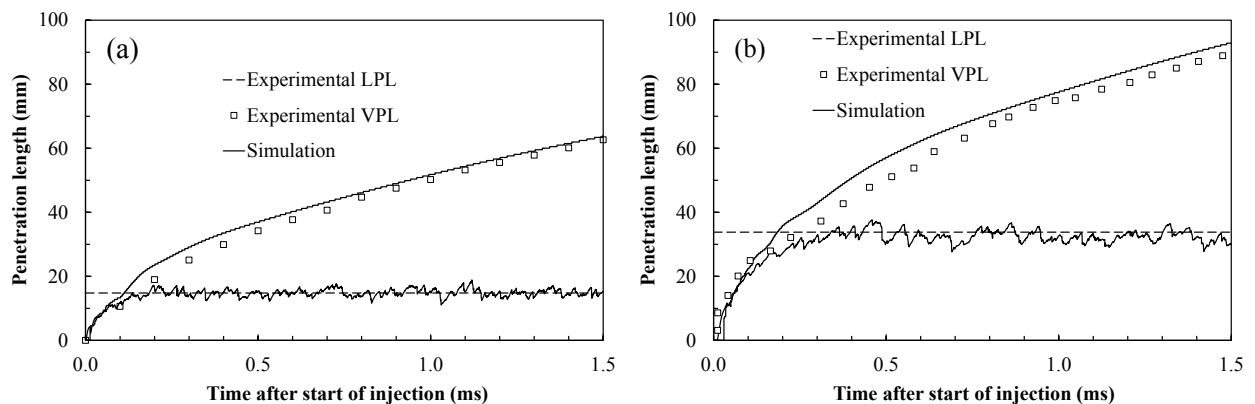


Fig. 1. Comparisons of experimental and simulated penetration lengths for the nozzle diameters of (a) $100 \mu\text{m}$ and (b) $257 \mu\text{m}$. Note that the experimental LPL is produced using the liquid length scaling law [13].

The experimental LPL and VPL data for the 100 μm nozzle diameter case are collected from Refs. [13] and [1] respectively. It should be mentioned that, the VPL measurement for the non-reacting diesel spray for the 100 μm nozzle diameter case is not available. Hence, that of *n*-heptane is used to evaluate the model, assuming that the VPL evolution is independent from fuel types [17]. Considering that non-reacting spray measurements for the 180 μm and 363 μm nozzle diameter cases are not available, an intermediate nozzle diameter of 257 μm is used in the current work to evaluate the model performance in simulating the non-reacting spray of large nozzle diameters. For LPL, the comparison is made against the LPL determined with the liquid length scaling law [13]; while the VPL results are compared with the measurement reported by Naber and Siebers [14]. Comparisons of experimental and simulated penetrations lengths are provided in Figure 1. As illustrated, the numerical models are capable to replicate the experimental LPL and VPL reasonably well. It is also noted that the relative change of LPL and VPL with respect to the change of nozzle diameter is reproduced by the model.

3.2. Reacting sprays

Figure 2(a) illustrates the averaged pressure rise in the three reacting cases (cases 3 to 5). The IDT is defined as the time where the steepest pressure rise is recorded. As shown, the IDT values do not vary significantly when the nozzle diameter is increased from 100 μm and 180 μm . A minor increase in IDT is observed only when a larger nozzle diameter is used. These trends are reproduced by the current model and the relative differences in IDT remain below 28%. The model also predicts that a higher rate of averaged pressure rise is produced in the case with a larger nozzle diameter and a greater fuel mass flow rate. Figure 2(b) shows the averaged LPL and LOL as a function of nozzle diameter. The LOL is defined as the length between the injection tip and the location where OH mass fraction of 4×10^{-4} is first observed. Despite the IDTs are similar, the LOL increases with the nozzle diameters. A maximum difference of 13% is obtained for the prediction of LOL. The averaged LPL in the reacting cases also increases with the nozzle diameter. The associated dependence on nozzle diameter is much stronger, as compared to that of LOL. This significantly influences the air entrainment and the flame structure (see below).

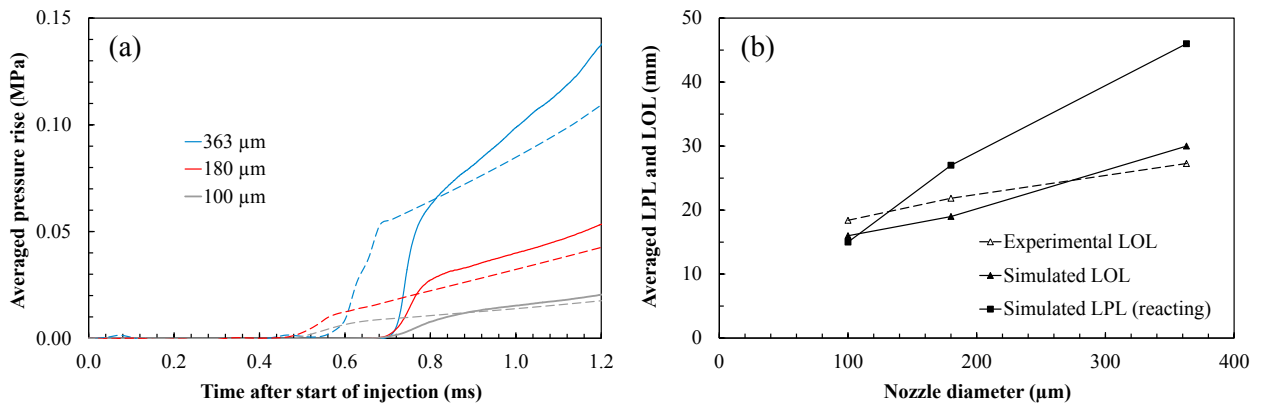


Fig. 2. Comparisons of experimental and simulated (a) averaged pressure rise as well as (b) LPL and LOL for different nozzle diameters. In (a) the dashed lines are experimental results while the solid lines are numerical predictions.

Figure 3(a) shows the comparisons of temperature-equivalence ratio (T - ϕ) scatter plots for the three established flames, which are extracted at approximately 0.5 ms after their respective IDTs. Although the ϕ value within the rich premixed core for a given nozzle diameter usually decreases with the increase of LOL due to the stronger air entrainment, an opposite trend is observed here. The spray flame from the larger nozzle diameter has a richer fuel region within the region of local temperature of 1200 K to 2200 K, indicating that the amount of air entrained into the upstream of the flame is more strongly affected by the amount of fuel being injected and the averaged LPL than by the LOL. The higher ϕ values agree with the rise of soot concentration measured in the cases with larger nozzle diameters [16]. Figure 4 depicts the temperature contours for the established flames. Black solid lines are used to represent iso-contours of ϕ ranging from 1 to 4, where $\phi=1$ denotes the stoichiometric mixtures (*st*). As shown, the

centre of the spray jets are cooled by the vaporised fuels and have rather low temperatures. The low temperature region is extended with the increase of nozzle diameter. When the nozzle diameter of 363 μm is used, the fuel-rich regions mainly appear to be adjacent to the stoichiometric mixtures and do not meet along the spray axis prior to flame impingement on the chamber wall.

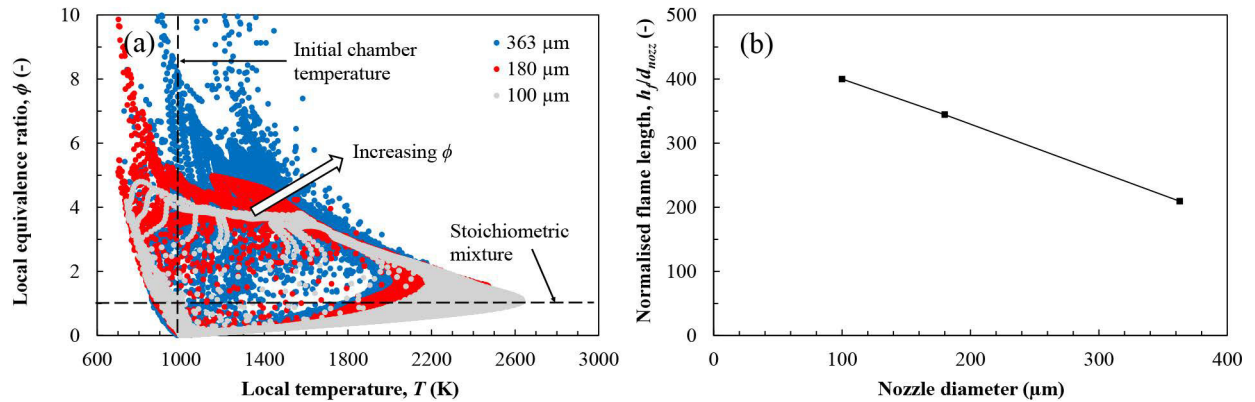


Fig. 3. Comparisons of (a) T - ϕ characteristics and (b) normalised flame lengths for different nozzle diameters.

Flame lengths of diesel fuel jets have received little attention since impingement of spray flames on piston bowls and/or cylinder liners occur prior to the establishment of the spray flames in practical automotive engine situations. However, the cylinder bores of marine engines are larger. The spray flame jets, particularly those of large, two-stroke marine engines can somewhat be formed [18]. In the case of multiple injections, the flame jet formed in the first fuel injection is expected to affect the ignition and combustion of the subsequent fuel injection. Figure 4 illustrates the flame structures at approximately 0.5 ms after their respective IDTs. It is apparent that the flame development progresses more rapidly and the spray flame jets are longer (and wider) in the cases with larger nozzle diameters. For quantitative comparisons, the flame length is defined as the length where a significant amount of OH mass fraction is observed. The threshold is set to 4×10^{-4} , which is similar to the definition used for LOLs. The associated iso-contours are represented by the white solid lines. The simulated flame lengths (h_f) are then normalised by the orifice diameters (d_{nozz}). The normalised flame length, as shown in Figure 3(b), appears to decrease as the orifice diameter increases. The trend qualitatively agrees with the experimental measurements which were obtained for smaller nozzle diameters (ranging from 50 μm to 100 μm) under the same thermochemical condition [16].

4. Conclusions

The current study demonstrates that the ESF model successfully replicates important spray flame features when various nozzle diameters are used. For the tested nozzle diameters which range from 100 μm to 363 μm , maximum relative differences of 28% and 13% are obtained for the IDT and LOL respectively. The simulation results also show that the local equivalence ratio within the rich premixed core increases with larger nozzle diameters. This agrees with the rise of soot concentration inferred by the soot incandescence measurements [16]. The simulated normalised flame length is found to decrease when the nozzle diameter increases. This trend qualitatively agrees with the experimental measurements obtained for smaller nozzle diameters which range from 50 μm to 100 μm [16]. The validated model is expected to serve as a prerequisite to simulate the ignition and combustion in marine engines where fuel injectors with different nozzle diameters are used for pilot and main injections.

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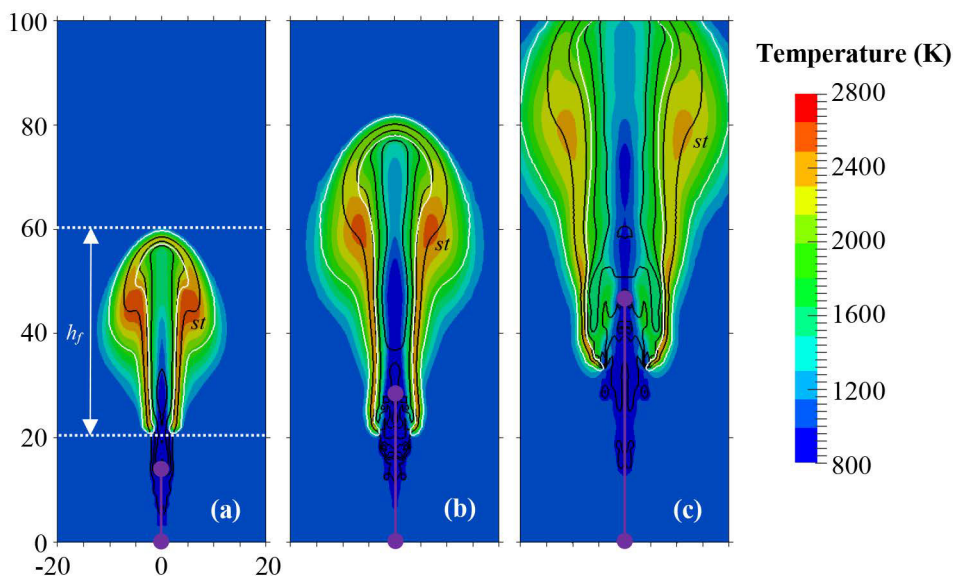


Fig. 4. Comparisons of temperature distributions of the established flames for nozzle diameters of (a) 100 μm , (b) 180 μm and (c) 363 μm . The temperature contours, equivalence ratio iso-contours (black lines) and OH mass fraction iso-contours (white lines) are reflected along the spray axis; while the purple solid lines represent the averaged LPL in the reacting cases.

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