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Large-eddy simulation on the influence of injection pressure in reacting Spray A

Heikki Kahila[a,*], Armin Wehrfritz[a], Ossi Kaario[a], Mahdi Ghaderi Masouleh[a], Noud Maes[b], Bart Somers[b], Ville Vuorinen[a]

[a] Department of Mechanical Engineering, Aalto University School of Engineering, Puumiehenkuja 5, Espoo 02150, Finland
[b] Department of Mechanical Engineering, Eindhoven University of Technology, Den Dolech 2, Eindhoven 5612 AZ, The Netherlands

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ABSTRACT

The Engine Combustion Network (ECN) Spray A target case corresponds to high-pressure liquid fuel injection in conditions relevant to diesel engines. Following the procedure by Wehrfritz et al. (2016), we utilize large-eddy simulation (LES) and flamelet generated manifold (FGM) methods to carry out an injection pressure sensitivity study for Spray A at 50, 100 and 150 MPa. Comparison with experiments is shown for both non-reacting and reacting conditions. Validation results in non-reacting conditions indicate relatively good agreement between the present LES and experimental data, with some deviation in mixture fraction radial profiles. In reacting conditions, the simulated flame lift-off length (FLOL) increases with injection pressure, deviating from the experiments by 4–14%. Respectively, the ignition delay time (IDT) decreases with increasing injection pressure and it is underpredicted in the simulations by 10–20%. Analysis of the underlying chemistry manifold implies that the observed discrepancies can be explained by the differences between experimental and computational mixing processes.

1. Introduction

Modern compression-ignition engines aim towards fuel lean, low-temperature combustion (LTC) in order to reduce soot and NOx emissions [1]. In direct injection engines, the fuel is supplied into the engine cylinder by a high-pressure injection system. To optimize the system, the nozzle hole size and shape, number of holes, injection timing or the injection pressure can be adjusted. Supplementary to the injection strategy, the ambient temperature, density and oxygen concentration are important, for instance, when reducing emissions by means of exhaust gas recirculation (EGR). Understanding the complex multiscale physics and chemistry of fuel sprays is essential in order to better control and improve the combustion process.

In compression-ignition direct injection engines the fuel droplets atomize and vaporize forming a high-speed gaseous fuel jet. Such a high-speed jet introduces strong shear, producing turbulence and enhancing fuel-oxidizer mixing. Once the temperature of the compression process exceeds the autoignition temperature and sufficient mixing has ensued, local regions with the most favorable conditions will ignite. The time from the start of injection (SOI) to ignition is referred to as the ignition delay time (IDT). Directly after the ignition, the flame front expands in three dimensions and forms a quasi-stationary diffusion flame. The diffusion flame stabilizes to a specific distance downstream from the injector, commonly referred to as the flame lift-off length (FLOL). It is worth noticing that the FLOL and IDT both depend on the injection parameters and the ambient conditions described in the previous paragraph [2].

Recent advances in computational resources have enabled large-eddy simulations (LES) of spray flames with high resolution and complex chemical schemes for realistic surrogate fuels. However, numerical model validation requires well defined experimental conditions and for spray flames this has been made possible by the Engine Combustion Network (ECN) [3]. The ECN provides an open-access data repository and a forum for international experimental and numerical collaboration. Baseline target conditions with guidelines for the diagnostic/post-processing techniques have been defined by the ECN for different spray cases. In particular, this study is involved with the ECN *n*-dodecane spray combustion case, designated as Spray A with the following target conditions: ambient gas temperature is 900 K, ambient pressure is approximately 6 MPa and the molar oxygen concentration is 15%.

* Corresponding author.
E-mail address: heikki.kahila@aalto.fi (H. Kahila).

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The injection system has a 150 MPa rail pressure with a nominal nozzle hole diameter of 90 µm. Several experimental studies have been carried out for the non-reacting and reacting Spray A case at different ambient conditions and with different injection pressures [3–9].

The experimental results [3–9], regarding the injection pressure variation, indicate a weak sensitivity of liquid penetration on the injection pressure (see also [10]). In contrast, vapor penetration was found to increase with injection pressure due to the increased momentum of the evaporated fuel. In reacting conditions, the IDT was found to be inversely proportional to the injection pressure, whereas the FLOL was noted to be directly proportional to the injection pressure [3,5,6]. Increase in FLOL with higher injection pressures for different surrogate diesel fuels (not Spray A) has also been reported [11,12].

Computational Spray A studies on injection pressure effects have been previously conducted only in the Reynolds-Averaged Navier–Stokes (RANS) framework. Banerjee et al. [13] reported overpredicted ($\sim$20%) IDT and FLOL by RANS and multi-flamelet representative interactive flamelet (RIF) models. Pei et al. [14] applied RANS and the transported probability density function (TPDF) combustion model for the 50, 100 and 150 MPa injection pressures, with numerical results agreeing with the experiments in terms of FLOL but overpredicting the IDT by $\sim$25%. In general, Spray A related RANS studies have been performed with a variety of different combustion models, including the well mixed combustion model, RIF model [15,16] and the TPDF model [14,17].

In the LES context, Spray A has been previously studied with different combustion models. Gong et al. [18,19] applied the chemistry coordinated mapping (CCM), whereas Pei et al. [20] utilized LES and finite rate chemistry at various ambient temperatures and indicated the relevance of ignition kernels as a flame stabilization mechanism. Blomberg et al. [21] applied the conditional moment closure (CMC) methodology in the split injection Spray A case obtaining good agreement with the experiments in terms of IDT and spatial appearance of low-temperature combustion species, including CH_2O. Recently Hakim et al. [22] used the Bayesian inference calibrated 2-step mechanism together with the dynamic thickened flame model to study the real gas effects and turbulence–chemistry interaction (TCI) on the ignition.

When considering accuracy of the combustion model, CMC [21,23], TPDF [14,24] and finite rate chemistry [20] approaches have provided results which agree well with the experiments. In particular, performance of CMC and TPDF in TCI modeling is notable. In contrast to these computationally demanding methods, another modeling avenue is given by flamelet-based methods, where lookup-tables are computed beforehand to reduce computational overhead [25,26]. Previously, flamelet based methods have been applied to spray combustion under engine like conditions, e.g. by Ameen and Abraham [27] in terms of the unsteady flamelet progress variable (UFPV) model, and by Bekdemir et al. [28] and Tillou et al. [29] with the FGM model. Recently, Wehrfritz et al. [30] applied the FGM model in the Spray A case at different ambient oxygen concentrations. These studies show how the tabulation method can capture the ignition and flame characteristics of the complex non-premixed spray combustion process.

In addition to the choice of the combustion model, the underlying chemical mechanism can vastly influence the results. For example, Wehrfritz et al. [30] showed a consistent offset between the mechanism by Ranzi et al. [31] (130 species) and Narayanaswamy et al. [32] (257 species) within the same LES-FGM framework. Pei et al. [20] attributed their IDT overprediction at low ambient temperatures to the lack of accuracy in the chemical mechanism by Luo et al. [33] (103 species). Other examples of mechanisms applied in LES Spray A context are the mechanism by Som et al. [34] (103 species) in the LES-CCM work by Gong et al. [18] and the mechanism by Yao et al. [35] (54 species) in the recent LES-CMC work by Blomberg et al. [21].

Spray sub-models are also considered as an important aspect in spray combustion simulations. Typically in engine conditions, the fuel spray poses a short liquid core, due to rapid atomization and evaporation. Therefore, the atomization process is modeled by applying a certain initial droplet size distribution, whereas the secondary droplet breakup is taken into account by sub-models [36]. A thorough literature review related to the challenges in Lagrangian–Eulerian coupling is presented in Ref. [37]. As implied by the literature, the LPT-LES has become a major tool for investigating turbulent spray flames, with varying sub-models [17,18,20,38–40].

Based on the previous literature, there are a number of unexplored questions in the combustion physics of spray diffusion flames and particularly in computational modeling of the ECN Spray A. In this study we continue our previous work on the LES-FGM based Spray A research [30] and formulate the objectives as follows:

1. Compare the computational fuel-oxidizer mixing process in non-reacting conditions with the available experimental data for 50, 100 and 150 MPa injection pressures.
2. Compare the computationally obtained IDT and FLOL with the available experimental data for 50, 100 and 150 MPa injection pressures.
3. Study the potential of the present unsteady flamelet based combustion model to reach a level of detail in low-temperature combustion phenomena and flame stabilization mechanisms equivalent to previous literature (see Pei et al. and Skeen et al. [9,20]).
4. Determine how the size of the low-temperature combustion region is affected by the change in injection pressure.
5. Explain the similarities and discrepancies between different injection pressures from a) the LES modeling and b) from the FGM tabulation perspectives.

The paper is organized as follows: The computational theory and numerical details are provided in Section 2. The computational and experimental set-up is described in Section 3. The results of the non-reacting and reacting cases are analyzed in Sections 4.1 and 4.2, respectively. Further analysis of the reacting results is carried out in Sections 4.3–4.8. A summary and conclusions are given in Section 5.

2. Numerical methods

2.1. Gas phase governing equations

The Eulerian gas phase is described by the compressible Navier–Stokes equations. The Favre-filtered LES formulation for the continuity, momentum and energy equations is the following:

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \overline{\rho}\widetilde{u_i}}{\partial x_i} = \overline{S_\rho}, \tag{1}$$

$$\frac{\partial \overline{\rho}\widetilde{u_i}}{\partial t} + \frac{\partial (\overline{\rho}\widetilde{u_i}\widetilde{u_j})}{\partial x_j} = \frac{\partial}{\partial x_j}\left(-\overline{p}\delta_{ij} + \overline{\rho}\widetilde{u_i}\widetilde{u_j} - \overline{\rho}\widetilde{u_i}\widetilde{u_j} + \overline{\tau_{ij}}\right) + \overline{S_{u,i}}, \tag{2}$$

$$\frac{\partial \overline{\rho}\widetilde{h_t}}{\partial t} + \frac{\partial (\overline{\rho}\widetilde{u_j}\widetilde{h_t})}{\partial x_j} = \frac{\partial \overline{p}}{\partial t} + \frac{\partial}{\partial x_j}\left(\overline{\rho}\widetilde{u_j}\widetilde{h} - \overline{\rho}\widetilde{u_j}\widetilde{h} + \frac{\overline{\lambda}}{\overline{c_p}}\frac{\partial \widetilde{h}}{\partial x_j}\right) + \overline{S_h}, \tag{3}$$

where $\overline{\rho}$, $\widetilde{u_i}$, $\overline{p}$, $\widetilde{h}$, $\overline{\tau_{ij}}$, denote the filtered density, velocity, pressure, absolute enthalpy and viscous stress tensor, respectively. In particular, the overbar denotes an unweighted ensemble average, whereas the tilde ($\sim$) denotes a density-weighted ensemble average. Variables $\overline{c_p}$ and $\overline{\lambda}$ denote the heat capacity and conductivity.