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Large Eddy Simulation of *n*-dodecane spray flames using Flamelet Generated Manifolds

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ABSTRACT

In the present study the Engine Combustion Network (ECN) "Spray A" target conditions are investigated using the Large Eddy Simulation (LES) and the Flamelet Generated Manifold (FGM) methods. We investigate *n*-dodecane spray flames at three different ambient oxygen levels in engine relevant conditions. The flamelet database is generated by simulating the counterflow diffusion flamelets for two recently developed *n*-dodecane mechanisms with 257-species/1521-reactions (Narayanaswamy et al., 2014) and 130-species/2395-reactions (Ranzi et al., 2014). In addition to validation in non-reacting conditions, we evaluate the performance of the newly implemented FGM model by comparing spray ignition delay times and flame lift-off lengths to the available experimental data within the ECN. The obtained ignition delay times agree well with the experimental data for the mechanism by Ranzi et al., 2014 and are over-predicted for the mechanism by Narayanaswamy et al., 2014. This observation is consistent with a respective trend in the observed flame lift-off lengths. Further, we provide evidence of only minor spray realization to realization variation of the ignition delay time in the present configuration. The spray flame structure is noted to consist of two parts: (1) a diffusion flame enveloping the combusting part of the spray close to the stoichiometric isoline, and (2) a premixed combustion regime in the fuel-rich core of the spray. During spray ignition, the model predicts the spatio-temporal phases of ignition. The model also indicates the presence of a 'cool flame' between the flame lift-off length and the nozzle. For the first time, we quantify the size of such a topological structure. In general, the flamelet data showed significant differences in the ignition characteristics between the two chemical mechanisms for all three ambient oxygen cases, but indicated little differences for a steady flame.

1. Introduction

Reacting high-velocity fuel sprays comprise an important and challenging topic in turbulent combustion research. Spray combustion systems can be found in many practical applications, such as industrial burners, aircraft combustors, or internal combustion engines. The main topic in the present paper is the fuel spray flame in a direct injection diesel engine. In such engines a liquid fuel jet is injected into hot ambient air undergoing rapid atomization, evaporation, turbulent mixing and combustion. Considering the essential linkage between fuel spray flames, engine heat release, and emissions, diesel sprays in reacting and non-reacting conditions have been under extensive experimental and computational investigations in the past.

Diesel sprays are characterized by a non-premixed liquid fuel injection configuration. The conventional picture of a diesel spray flame consists of a high temperature diesel flame in which the combustion process is primarily mixing controlled. However, despite the non-premixed introduction of the liquid fuel, diesel flames are known to exhibit both, a fuel-rich premixed combustion regime and a non-premixed diffusion flame [3,4]. Key aspects in diesel spray combustion are autoignition and flame lift-off. The autoignition time determines the heat release phasing, whereas the flame lift-off is essentially a measure for the flame stabilization and of key importance with respect to emission formation. In contrast to conventional diesel combustion, modern diesel engines often aim at low temperature combustion (LTC) [5] to reduce harmful emissions. This objective could be reached via a more homogenous mixture formation or a dilution of the fuel–air mixture through the recirculation of exhaust gases. In fact, the present study is strongly motivated by the modern combustion concepts aiming at control of ambient oxygen levels. Such scenario is expected to somewhat change the conventional high temperature diesel combustion picture and introduce a stronger dependency on the chemical processes.

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The broad range of length and time scales, in combination with the multiphysics nature of turbulent spray combustion, imposes various challenges to experimental and computational research. Direct Numerical Simulation (DNS) of high-velocity fuel sprays will remain computationally prohibitive for several decades to come [6]. However, recent DNS work on engine relevant spray and combustion configurations have further contributed to the understanding of the autoignition process, even though the studies have been limited to strongly simplified configurations [7–11]. Large Eddy Simulation (LES) methods, on the other hand offer a versatile tool for turbulent combustion research and have been successfully used in a wide range of single phase reacting flows. The application of LES for turbulent spray combustion simulation has increased in the recent years (e.g., [12–17]), mainly due to the progress in modeling of the various subgrid scale processes related to droplets, turbulence, mixing and combustion [17–24].

In order to develop and validate advanced computational models with the goal to establish predictive modeling capabilities, well defined and accurately measured experimental data are necessary. In a similar manner as in the series of workshops on Turbulent Nonpremixed Flames (TNF) [25], where accurate and extensive experimental data were used to validate canonical atmospheric jet flames, the Engine Combustion Network (ECN) [26] was established for collaboration on turbulent spray flames under engine operating conditions. While the two collaborative efforts share the same principles, significant differences can be found in the physical and chemical conditions. For instance, the large injection velocity of liquid fuel in diesel engines (typically in the order of 500 ms^{-1}) results in a high momentum jet, which subsequently leads to a substantially larger flame lift-off for diesel spray flames compared to laboratory jet flames. Also the elevated ambient pressure and the long chained hydrocarbon fuels are important differences, which show the need for well defined measurements under conditions relevant to diesel engines.

The chemical composition of commonly available diesel fuel is complex and hence its thermodynamical and chemical properties are difficult to access. In order to accurately define the fuel properties for experimental and computational combustion research, surrogate fuels, such as the Primary Reference Fuels (PRF) for gasoline [27], are widely used. Diesel fuels have been represented by *n*-heptane in a wide range of experimental [28–30] and computational studies [12,15,31–41] and hence also the first target conditions within the ECN were using *n*-heptane. A particular advantage of *n*-heptane is the availability of tractable and widely tested chemical mechanisms; comprehensive lists of *n*-heptane studies can be found in [36,37]. However, the carbon chains of typical diesel fuel components range from 10 to 25 carbon atoms [42] and hence the thermophysical properties, especially with respect to evaporation and boiling, are not well represented by *n*-heptane. As a more suitable surrogate for diesel fuel, *n*-dodecane was identified due to the longer carbon chain and the well defined thermophysical and transport properties [42]. A set of target conditions using *n*-dodecane, named *Spray A*, was defined to study canonical spray flames within the ECN [43,44]. Extensive experimental data for Spray A are available, including parametric variations for ambient temperature, density and oxygen concentration as well as injection pressure [45–50]. Several modeling studies of the Spray A case have been carried out, using various turbulence and combustion modeling approaches. However, the lack of accurate and yet computationally affordable chemical mechanisms for *n*-dodecane has been identified as a key issue and is still subject to ongoing research by several groups.

Recently, Luo et al. [51] developed and validated a skeletal *n*-dodecane mechanism with 106-species and 420-elementary reactions. The validation specifically targeted Spray A conditions, including three-dimensional spray simulation using unsteady Reynolds averaged Navier Stokes (RANS) turbulence modeling. This mechanism was also used by D'Errico et al. [52] comparing a well-mixed and the multiple Representative Interactive Flamelet (mRIF) combustion model for different ambient temperatures and oxygen concentrations of the Spray A conditions. The study employed a RANS based solver and in case of the mRIF model a presumed Probability Density Function (PDF) turbulence-chemistry interaction approach was used. It was found that generally a better agreement with experimental results was achieved for the mRIF model compared to the well-mixed model. A more comprehensive study with respect to Spray A parameter variation was conducted by Kundu et al. [53] using the same RANS/mRIF approach. Several presumed PDFs were investigated and the mechanism by Luo et al. was compared to an earlier version with 103-species and 370-elementary reactions by Som et al. [54]. The latter mechanism was also used by Bhattacharjee and Haworth [37] in a parameter study for the Spray A case using a two-dimensional RANS approach in combination with a Transported Probability Density Function (TPDF) method to model the reaction-diffusion processes. Similarly, Pei et al. [55] carried out a comprehensive parameter study of the Spray A conditions using a further reduced version of the mechanism by Luo et al., leading to 88-species. For the turbulence and reaction-diffusion modeling a two-dimensional RANS/TPDF approach was employed. In fact, most of the computational studies of spray combustion within the ECN have been based on the unsteady RANS approach with various combustion models.

The majority of the computational Spray A studies report ignition delay times and lift-off length predictions, but detailed investigations of spray ignition characteristics have mainly been carried out for *n*-heptane sprays. Most notably, the studies by Bhattacharjee and Haworth [15,37,38] investigated *n*-heptane spray ignition and provide a detailed analysis of ignition location and mixture conditions. The reasoning behind this can be mainly attributed to the widely tested chemical mechanisms for *n*-heptane and the uncertainties in the mechanisms used in the previous *n*-dodecane spray studies [37,56]. One of the few LES studies of the ECN target conditions, and specifically of Spray A, employs a chemistry coordinated mapping (CCM) method and the 103-species mechanism by Som et al. to model spray combustion [56]. Very recently, Pei et al. [16] utilized LES and finite rate chemistry in to investigate the effect of multiple realizations for the Spray A conditions at various temperatures. Hence, further investigations on Spray A at various ambient conditions using LES are required in order to better explore the spatio-temporal characteristics of ignition and combustion in *n*-dodecane spray flames.

In the present paper, LES of turbulent spray combustion is carried out using Lagrangian Particle Tracking (LPT) to model the liquid phase and the Flamelet Generated Manifold (FGM) [57] combustion model to account for the complex chemical reactions. As simulation platform we choose an open-source CFD code OpenFOAM into which the FGM model was implemented. The simulated spray cases correspond to the Spray A target conditions and the work extends the previous studies on high-velocity fuel sprays within the ECN. To quantify the influence of the chemical kinetics, two recently developed mechanisms are compared: (1) the 257-species/1521-reactions mechanism by Narayanaswamy et al. [1] (hereafter referred to as Stanford mechanism) and (2) the 130-species/2395-reactions mechanism by Ranzi et al. [2] (referred to as POLIMI mechanism). To the authors best knowledge, this is the first LES study of a high-velocity *n*-dodecane fuel spray to employ such detailed chemical mechanisms.

The present paper has four main objectives which address certain unexplored characteristics of the Spray A case using the implemented FGM model and LES. (1) The first objective is to

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