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Research Paper

Application of an unsteady flamelet model in a RANS framework for spray A simulation

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HIGHLIGHTS

- The spray A experiment from ECN is modeled by means of USFM.
- Satisfactory results are obtained for ID and LOL for parametric sweeps.
- Autoignition spatial location analyzed with temperature and mixture fraction fields.
- Remarkable similarity between modeled and experimental species fields.

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ABSTRACT

In the present investigation the Spray A reference configuration defined in the framework of the Engine Combustion Network (ECN) has been modeled by means of an Unsteady Flamelet Model (USFM) including detailed parametric studies to evaluate the impact of ambient temperature, oxygen concentration and density. The study focuses on the analysis of the spray ignition delay, the flame lift-off length and the internal structure of the spray and flame according to the experimental information nowadays available for validating the results provided by the model.

Promising results are obtained for the nominal case and also for the parametric variations (temperature, oxygen...) in terms of liquid and vapor penetration, ignition delay (ID) and lift-off length (LOL). The model permits to predict the ID and the LOL which constitute two parameters of key importance for describing the characteristics of transient reacting sprays. Valuable insight on the details of the combustion process is obtained from the analysis of formaldehyde (CH_2O), acetylene (C_2H_2) and hydroxide (OH) species in spatial coordinates and also in the so-called $\phi - T$ maps. Important differences arise in the inner structure of the flame in the quasi-steady regime, which is closely linked to soot formation, when varying the ambient boundary conditions. Additionally, the auto-ignition process is investigated in order to describe in detail the spatial onset and propagation of combustion. Results confirm the impact of the ambient conditions on the regions of the spray where start of combustion takes place, so the relation between the local scalar dissipation rate and mixture fraction variance is also discussed. This investigation provides an insight of the potential of the USFM combustion model to describe the physical and chemical processes involved in transient spray combustion.

1. Introduction

During the last decades the increasing interest for improving combustion efficiency and decreasing pollutant emissions in diesel engines highlighted the needs of achieving a better understanding of the combustion process in transient sprays. However, due to the great variety of physical and chemical phenomena involved in these complex problems, with so different time and length scales, this is still a challenging topic. Experimental measurements have historically provided the cornerstones of the knowledge on basic processes that occur in diesel sprays. In addition to experimental data and more recently, Computational Fluid Dynamic (CFD) modeling has arisen as a very powerful tool that enables to investigate the inner structure of diesel sprays providing valuable knowledge that has lead to important progress in applied combustion science [1–3].

Nevertheless, practical reasons sometimes impose strong hypotheses in the models in order to maintain a limited computational time that introduce additional uncertainties along the

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modeling workflow. In this sense both experimental and modeling activities are complementary and permit together to figure out the different aspects of the problem.

Following this approach, the Engine Combustion Network (ECN) [4] provides a large database with high-quality experimental results generated at different international institutions [5–7]. One of the most valuable aspects of these experiments is that they are carried out under well-defined and controlled conditions, discarding a great amount of the inherent uncertainties related to measurements in industrial devices.

Together with the experimental database great modeling effort has been devoted to evaluate and improve the CFD combustion models by performing numerical experiments. These simulations have the ability to reproduce the internal processes of the spray, providing in general good qualitative and in some cases also quantitative results in terms of ignition delay (ID) and lift-off length (LOL) compared to the available experimental data [8,9]. Additionally, the structure of the flame in terms of temperature, species and velocity fields has been a matter of interest in the modeling area and has encouraged the comparison of different models for providing suitable descriptions of the flame [10–12].

In the last times attention has been focused on the so-called spray A where n-dodecane is used as a diesel surrogate fuel. Boundary conditions span over a wide range and special emphasis is devoted to those conditions related to low temperatures and moderate EGR corresponding to the framework of combustion in modern diesel engines. Such boundary conditions are challenging for modeling because of the strong turbulence-chemistry interaction (TCI) [10].

Global parameters of the reactive flow such as ignition delay (ID) and lift-off length (LOL) together with the spray penetration and liquid length are indicators of major relevance that are systematically analyzed in reactive spray simulations in order to determine the predictive performance of models. Together with these parameters optical techniques, such as planar laser-induced fluorescence (PLIF) and high-speed schlieren imaging, permit to describe the transient evolution of the reacting spray and its internal structure by tracing the species spatial position during the combustion onset and development [13]. This provides new data for validating qualitatively the models in terms of their capability for reproducing the temporal-spatial reacting spray structure.

Several institutions have experimentally characterized spray A with different facilities that can be classified in constant-volume pre-burn (CVP) combustion vessels and constant-pressure flow (CPF) rigs [6]. A CPF experimental facility is available at CMT-Motores Térmicos and the database generated in this facility is used along this research [6,14,15].

Although spray A boundary conditions permit to investigate the internal flame structure and check the capability of the models, diesel engine simulations encompass a great variety of conditions and it is a requirement for the models to have the ability to yield acceptable results in these conditions with limited computational times. Between the different models that provide good results for industrial configurations the flamelet model in conjunction with tabulated chemistry has demonstrated to be one of the most powerful for premixed and non-premixed turbulent combustion modeling [16–19]. In such models flamelet look-up tables, which save the chemistry evolution in laminar flames, are generated previous to the CFD computation reducing drastically the computational time. Based on the satisfactory results provided for diesel engines by the Unsteady Flamelet Model (USFM) [20,21] together with Intrinsic Low Dimensional Manifolds (ILDM), a similar approach has been adopted for this work.

In particular, the Approximated Diffusion Flamelet (ADF) model [22] proposed some years ago for managing complex chemical mechanisms keeping a low computational cost has been used in this work to generate the laminar flamelet manifolds. The ADF model has been extensively validated including non-premixed laboratory flames [23,24] and diesel engine simulations [25,26], providing satisfactory results in all cases. The major advantage of the ADF model is then its suitability for generating the laminar flamelet manifolds in a very short time (few hours) even using complex chemical mechanisms.

As a main objective, this work investigates the spray A auto-ignition and combustion processes for the reference boundary conditions and also for parametric variations of ambient temperature, oxygen concentration and density. This study includes the description of the trends followed by the ID and LOL and additionally the analysis of the most relevant species fields in spatial coordinates and also in the intrinsic non-premixed combustion coordinates defined by the local equivalence ratio (ϕ) and temperature (T), which define the so-called ϕ-T maps widely used in spray combustion analysis. The modeling results will be compared with the available experimental data to evaluate the performance of the model. Thus, the paper starts by the methodology section, where the different spray and combustion models and the parametric studies carried out are described. The final model setup is defined and validated by comparing with experiments in non-reacting and reacting conditions. The next results and discussion section include the analysis of the global parameters, such as ID and LOL, followed by a dedicated discussion about the auto-ignition process and finally the reacting spray structure is described in detail. To close the paper the last section summarizes the main conclusions of the present investigation.

2. Methodology

2.1. Description of the model

The model was implemented in the open tool-box OpenFoam environment. A RANS (Reynolds Averaged Navier-Stokes) approach was used and cylindrical symmetry was supposed, i.e. the solution was obtained on a plane that corresponds to a meridian cut of a cylinder with a radius and a height equal to 54 mm and 108 mm, respectively. The mesh was structured with a constant cell size of 0.25 (radial direction) $\times$0.5 mm (axial direction) in the whole domain as suggested in [27].

A standard $k-\epsilon$ RANS turbulence model was selected adjusting $C_{\epsilon_1} = 1.52$ in order to correct the well-known round jet spreading overestimation of $k-\epsilon$ type models [28], which provides good results in spray simulations [29]. The other constants were kept at their standard values ($C_\mu = 0.09, C_{\epsilon_2} = 1.92, C_{\epsilon_3} = -0.33$, $\sigma_k = 1, \sigma_\epsilon = 1.3$).

The DDM (discrete droplet method) modeling approach has been adopted in this research work. The DDM comprises different sub-models that define the evolution of the spray liquid phase and its interaction with the gaseous carrier phase. In this work the atomization and breakup processes are described by modeling the Kelvin-Helmholtz/Rayleigh-Taylor instabilities. The values of the constants for the breakup and atomization models adopted for this work are $B_0 = 0.61, B_1 = 40, C_\tau = 1, CBU = 3$ as suggested in [27]. Additionally, the Ranz-Marshall model was selected for droplet evaporation with a multiplicative factor of 0.6 and exponents 0.5 and 1/3 for Reynolds and Prandtl numbers, respectively. Neither collisions nor coalescence models were included for the simulation of the spray. The number of parcels was chosen to be $5.4 * 10^7$ parcels/s.

The chemical mechanism used in this work to describe the dodecane chemistry corresponds to the Narayanaswamy et al. mechanism with 255 species and 2289 reactions [30].