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Importance of turbulence-chemistry interactions at low temperature engine conditions

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ABSTRACT

The role of turbulence-chemistry interaction in autoignition and flame stabilization is investigated for spray flames at low temperature combustion (LTC) conditions by performing high-fidelity three-dimensional computational fluid dynamics (CFD) simulations. A recently developed Tabulated Flamelet Model (TFM) is coupled with a large eddy simulation (LES) framework and validated across a range of Engine Combustion Network (ECN) ambient temperature conditions for n-dodecane fuel. High resolution grids with 0.0625 mm minimum cell size and 25 million total cell count are implemented using adaptive mesh refinement over the spray and combustion regions. Simulations with these grids and multiple LES realizations, with a 103 species n-dodecane mechanism show good agreement with experimental data for all the ambient conditions investigated. This modeling approach with the computational cost advantage of tabulated chemistry is then extended towards understanding the auto-ignition and flame stabilization at an ambient temperature of 750 K. These low temperature conditions lead to substantially higher ignition delays and flame liftoff lengths, and significantly leaner combustion compared to conventional high temperature diesel combustion. These conditions also require the simulations to span significantly larger temporal and spatial dimensions thereby increasing the computational cost. The TFM approach is able to capture autoignition and flame liftoff length at the low temperature conditions. Significant differences with respect to mixing, species formation and flame stabilization are observed under low temperature compared to conventional diesel combustion. At higher ambient temperatures, formation of formaldehyde is observed in the rich region (phi > 1) followed by the formation of OH in the stoichiometric regions. Under low temperature conditions, formaldehyde is observed to form at leaner regions followed by the onset of OH formation in significantly lean regions of the flame. Qualitative differences between species formation and transient flame development for the high and low temperature conditions are presented. The two stage ignition process is further investigated by studying the species formation in mixture fraction space by solving 1D flamelet equations for different scalar dissipation rates and homogeneous reactor assumption. Results show that scalar dissipation causes these radicals to diffuse within the mixture fraction space. This significantly enhances ignition and plays a dominant role at such low temperature conditions which cannot be captured by the homogeneous reaction assumption based model.

1. Introduction

Compression ignition engines will continue to play a dominant role in heavy duty applications due to their higher efficiency and power density. Considerable research effort has been directed towards improving their efficiency and reducing emissions. The traditional diesel engine strategy is characterized by mixing-controlled combustion and relatively high in-cylinder temperatures leading to a NOx-soot tradeoff. Reducing the overall temperature of combustion by employing lean mixtures has been the main strategy towards developing future engine concepts like Homogeneous Charge Compression Ignition, Premixed Charge Compression Ignition, Gasoline Compression Ignition and Lean Lifted Flame Combustion (LLFC) [1]. Autoignition at such conditions is a strong function of the chemical kinetics and turbulence-chemistry interactions. As a result, combustion phasing has proved to be a major challenge towards the development and application of these technologies. Numerical studies can be used as a tool to understand the mechanisms controlling the autoignition and flame stabilization processes resulting in an improved implementation of low temperature combustion strategies (LTC) in engines.

While a number of studies have been carried out in the recent past to understand the fundamentals of autoignition and flame stabilization at engine relevant temperature conditions, few studies

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have also focused on low temperature conditions that may be relevant towards future low-temperature engine concepts. Bansal et al. [2] studied auto-ignition of hydrogen-air premixed mixtures using two dimensional Direct Numerical Simulation (DNS) over a temperature range of 1033–1116 K. The mixtures were subjected to different levels of thermal and equivalence ratio stratification. The results show that ignition delay and heat release rate pattern have a strong dependency on the stratification. Mukhopadhyay and Abraham [3] modeled an n-heptane mixing layer at 40 bar pressure and 1000 K ambient temperature using two-dimensional DNS. Higher scalar dissipation rates in presence of higher compositional stratification led to an increase of ignition delay. In case of lower compositional gradients, higher scalar dissipation rates led to reduction in ignition delays. In a later study [4], the effect of heat release on evolution of scalar dissipation rate was studied. Borghesi et al. [5] carried out DNS of an igniting n-heptane spray at 24 bar pressure and 1000 K ambient temperature. Ignition kernels were observed in regions of lower scalar dissipation rate and mixture fractions corresponding to the most reactive mixture fraction from homogeneous reactor simulations. Krisman et al. [6] studied the two stage ignition process of a mixing layer with Dimethyl Ether (DME) and air at 40 atm and 900 K using 2D DNS. The study identified a cool flame propagation and its impact on high temperature ignition. It was observed that the high temperature ignition spots do not correspond to the most reactive mixture fraction obtained from the homogeneous reactor assumption. The first stage ignition was observed to be shorter, and, the cool flame propagates much faster into the rich regions as compared to the homogeneous reactor predictions. This is followed by the shortening of main ignition and formation of high temperature kernels. Thus, the scalar dissipation causes a reduction in the main, i.e., high temperature ignition delay for these conditions that are characterized by a two stage ignition, negative temperature coefficient (NTC) chemistry and low temperature chemistry. Dahms et al. [7] carried out similar studies in 1D flamelets and showed the influence of the first stage ignition on the main ignition. The analysis also showed the applicability of the flamelet concept for the entire ignition process for the Spray A conditions.

Three-dimensional DNS of a turbulent lifted DME jet flame at 5 atm ambient pressure by Minamoto and Chen [8] showed the influence of two stage ignition, NTC chemistry and turbulence-chemistry interactions on flame propagation and highlighted the need to account for turbulence-chemistry interaction (TCI) in Reynolds-Averaged Navier–Stokes (RANS) simulations and large-eddy simulations (LES). Borghesi et al. [9] extended this study to 3D DNS of n-dodecane mixing layers at an ambient pressure of 25 bar. Stratification of mixture fraction was shown to have a strong influence on low temperature reactions. For the parameters and thermodynamic conditions considered in their study, the scalar dissipation did not cause a reduction of the main ignition delay. This observation with respect to the main ignition was not same as that observed by Krisman et al. [6]. Dahms et al. [10] solved the 1D flamelet equations coupled with a detailed 2755 species n-dodecane mechanism [11] at the standard Spray A condition of the Engine Combustion Network (ECN) characterized by 60 bar and 900 K ambient pressure and temperature, respectively. Comparative 1D studies with homogeneous reactor ignition delays showed that increase in scalar dissipation rate reduces the ignition delay and shifts the ignition location to richer regions.

The fundamental studies using DNS illustrate the coupled effect of chemistry and turbulence on auto ignition and flame stabilization. The chemistry mechanisms also need to capture the two stage ignition process and predict the low temperature species. The diffusion and transport of these low temperature species have a significant influence on the main ignition process. However, such high fidelity studies cannot span the time scales, length scales and Reynolds numbers encountered in an actual engine due to their high computational costs. This motivates the use of LES to get an understanding of these processes in engines. LES of igniting n-dodecane sprays that mimic diesel engine conditions (ECN spray A) have been reported in some studies. Pei et al. [12–14] implemented a homogeneous reactor combustion model and a multi-zone framework along with a 103 species n-dodecane mechanism [15] within a LES framework over a range of ambient temperatures and oxygen concentrations [12]. A minimum grid size of 0.0625 mm with approximately 22 million cells was found to be sufficient for these conditions. A similarity index analysis was used to find out the minimum number of LES realizations that are required to obtain statistically converged predictions. Quantitative and qualitative data from the simulations matched the experimental measurements over the range of investigated conditions. Ameen et al. [16] showed that a combination of azimuthal and ensemble averaging can be used to reduce the total number of LES realizations. Wehrfritz et al. [17] implemented the Flamelet Generated Manifold (FGM) combustion modeling approach to model the ECN spray A over a range of oxygen concentrations with multiple realizations for the 15% oxygen condition and a single realization for the other conditions. A 0.0625 mm minimum cell size mesh near the nozzle with 11 million cells was used in this study. Two different n-dodecane chemistry mechanisms were compared with respect to autoignition, flame stabilization and species formation. Qualitative results showed good agreement between simulation and experiments with respect to formation of CH_2O. Flame liftoff length from simulations was over predicted for the higher oxygen concentration. Ameen et al. [18] recently implemented the Tabulated Flamelet Model (TFM) within the LES framework and validated it against different ambient temperature conditions for a single LES realization and compared the results against the homogeneous reactor combustion model for an ambient temperature range of 800 to 1100 K. The model was able to predict the autoignition and flame liftoff length trends accurately. Qualitative data showed the formation of ignition kernels and transient flame development and stabilization under engine conditions. The high fidelity LES simulations have been limited to the range of 800 to 1100 K ambient temperature conditions with single injection. The one notable exception is the recent study by Blomberg et al. [19] who carried out simulations of split injection at 900 and 750 K ambient temperatures using the CMC combustion model coupled with LES with a relatively coarse mesh and minimum cell size of 0.125 mm. The total simulation duration was 1.5 ms with each injection spanning 0.5 ms separated by a dwell time of 0.5 ms. The model was able to capture the soot formation, intermediate species and combustion recession accurately. The availability of spray flame diagnostics data under diesel-engine relevant conditions, courtesy of the ECN, has led to several LES studies of the ECN sprays [20–23]. These studies have greatly increased our understanding of the autoignition, flame development and flame stabilization mechanisms under these conditions. Although these LES studies provide slightly conflicting explanations regarding the flame stabilization mechanism for these spray flames, most of these studies are able to predict the flame lift-off lengths accurately despite using different TCI models. It could be hypothesized that if the LES setup is able to predict the flow and mixing field correctly, and the grid is sufficiently resolved, TCI only plays a minor role in determining the flame lift-off length. However, these observations may only not hold true for LTC conditions, where the ignition delays are long, and the turbulent diffusion of intermediary species can strongly affect the autoignition behavior.

Over the past years, a number of RANS simulations encompassing a variety of combustion models and chemistry mechanisms have been carried out to model igniting spray flames at diesel engine conditions. Pei *et al.* carried out RANS simulations using the