Direct Numerical Simulations of premixed methane flame initiation by pilot n-heptane spray autoignition

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ABSTRACT

Autoignition of n-heptane sprays in a methane/air mixture and the subsequent methane premixed flame ignition, a constant volume configuration relevant to pilot-ignited dual fuel engines, was investigated by DNS. It was found that reducing the pilot fuel quantity, increases its autoignition time. This is attributed to the faster disappearance of the most reactive mixture fraction (predicted from homogeneous reactor calculations) which is quite rich. Consequently, ignition of the n-heptane occurs at leaner mixtures. The premixed methane flame is eventually ignited due to heating gained by the pressure rise caused by the n-heptane oxidation, and heat and mass transfer of intermediates from the n-heptane autoignition kernels. For large amounts of the pilot fuel, the combustion of the n-heptane results in significant adiabatic compression of the methane–air mixture. Hence the slow methane oxidation is accelerated and is further promoted by the presence of species in the oxidizer stream originating from the already ignited regions. For small amounts of the pilot fuel intermediates reach the oxidizer stream faster due to the very lean mixtures surrounding the n-heptane ignition kernels. Therefore, the premixed methane oxidation is initiated at intermediate temperatures. Depending on the amount of n-heptane, different statistical behaviour of the methane oxidation is observed when this is investigated in a reaction progress variable space. In particular for large amounts of n-heptane the methane oxidation follows roughly an autoignition regime, whereas for small amounts of n-heptane methane oxidation is similar to a canonical premixed flame. The data can be used for validation of various turbulent combustion models for dual-fuel combustion.

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1. Introduction

Reciprocating engines is an important and growing area for natural gas utilization due to the lower NO_x, CO_2 and soot emissions achieved [1–3]. The small propensity of natural gas to autoignite allows high intake pressures and high compression ratios with turbochargers [1,3,4], which then allows high thermodynamic efficiencies [1,3,5]. Small natural gas engines are typically ignited by a spark [3,6]. However, large-bore engines as in power generation and the marine engine sector, where the pressure at the time of ignition is high, are typically ignited by a pre-chamber and a jet [7,8], or by a pilot injection of a liquid fuel which is easy to autoignite [1,3–5]. Essentially, the ignition centres of the pilot fuel provide the energy required for the initiation of the gaseous premixed flame [5,6,9–11]. This second mode of ignition, which involves autoignition of a pilot spray in a oxidiser that is already mixed with another fuel is studied in this paper from a fundamental perspective.

There is only limited work in the context of simulations and experiments for this complex problem. From a practical perspective, previous research has focused on rapid compression machines [11,12] and single cylinder four stroke direct injection engines [2,10,13,14]. One of the key findings was that ignition of the pilot spray is retarded in the presence of methane [2,11,12,14], and that OH* chemiluminescence intensity is increased, indicating an active role of methane in the combustion process [10,11]. It was also observed that increasing the number of holes in the liquid fuel injector enhances methane consumption [11,15] due to the larger number of the pilot fuel ignition centres that were available. In an effort to enhance the knowledge from the experimental observations various numerical approaches have been attempted aiming to model the combustion of a gaseous fuel mixed with air, ignited by the injection of a higher hydrocarbon fuel under engine relevant conditions [15–17], but there is very limited use of advanced turbulent combustion models. Schlatter et al. (2011) [16] used a two-dimensional Conditional Moment Closure (CMC) formulation and defined the hot spots predicted from the CMC model as the initial kernels of a premixed flame model [16]. However, since the ignition spots were simplified as premixed flame kernels,

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the exact mechanism causing the premixed methane flame initiation and the extent to which the flame is sustained was not examined. The structure of premixed flames in a conditioning-variable space, as in CMC, has been explored [18,19], but ignition of such flame through second fuel autoignition has not been studied.

The description of the combustion of a gaseous fuel in the presence of a higher hydrocarbon fuel poses another challenge, the choice of the chemical scheme to implement in order to model the simultaneous oxidation of both fuels. Various attempts have been reported in order to construct computationally viable mechanisms under engine relevant conditions; for example Khalil et al. (1996) examined a detailed scheme and derived a reduced scheme [9]. Conversely, Maghbouli et al. (2013) added oxidation paths of methane to an existing mechanism of higher hydrocarbon (n-heptane) in order to facilitate dual fuel investigations [17]. Schlatter et al. (2011) [16] used a chemical mechanism validated for n-heptane autoignition (pilot fuel) which contains methane [20], but it was not verified whether this can adequately describe the methane oxidation.

Apart from simulations based on RANS and the above-mentioned preliminary experiments there is no fundamental study of dual fuel combustion with two-phase turbulent combustion simulations. Direct Numerical Simulations (DNS) have proven to be a valuable tool for providing information on the autoignition and spark ignition of turbulent sprays [21–26]. Nevertheless the second fuel in the oxidiser is expected to alter the way autoignition kernels develop as reviewed in Ref. [27] and in greater extent the propagation in a gas-fuelled premixed mixture. The dual fuel combustion problem can also be thought of as an extension of the turbulent premixed flame problem in the sense that the hot kernel comes from liquid fuel autoignition rather than heat addition to a fluid of homogeneous composition [28,29]. Notwithstanding the information provided by DNS of turbulent spray combustion and premixed flame investigations, the dual fuel combustion case is characterised by complex flame structures featuring both non-premixed autoignition and premixed flames [30] and the fundamentals of these processes have not been studied in the necessary detail before [3].

The specific objectives of this work are: (i) to investigate the fundamentals of liquid fuel (n-heptane) autoignition in the presence of methane; (ii) to demonstrate how the autoignition of the n-heptane is affected by the amount of the liquid fuel; and (iii) to investigate the premixed methane flame initiation mechanism and how this is affected by the amount of n-heptane. This investigation is performed in the context of two phase DNS using complex chemistry. The pilot fuel quantity is varied while the temperature, turbulence intensity, and premixed methane equivalence ratio are kept constant.

2. Mathematical formulation

2.1. Overview

The details of the code and the governing equations have been described in previous works considering spark ignition of turbulent sprays [22,23] and autoignition of turbulent sprays under high pressures and intermediate temperatures [24,31]. Therefore, the governing equations for the liquid and gaseous phases are provided here as Supplementary Material for the interested reader for the purposes of completeness. In summary, the liquid phase consisted of n-heptane droplets and was treated with the Lagrangian point-source approximation assuming uniform temperature within the droplet. The droplet evaporation rate and the amount of heat exchanged with the gaseous phase were computed based on the thin film assumption [32]. The physical properties of the air/vapour mixture in the film were evaluated according to the 1/3 rule [33]. For each droplet a set of equations was solved in order to determine its position, velocity, diameter, and temperature [34]. The droplet Spalding numbers for heat and mass transfer appearing in the liquid phase governing

equations were evaluated according to [34] and are variable with time. Regarding the gaseous phase, fully compressible fluid is considered. The temporal and spatial evolution of the gaseous phase is described by the continuity of mass, momentum, internal energy, and $N_s - 1$ transport equations for conservation of species mass fraction, where N_s is the number of species for which transport equations are solved. The Lewis number is assumed to be equal to unity for all the species. The heat capacity and enthalpy for the species are evaluated using fifth order polynomials provided by [20]. In order to account for the changes in mass, momentum, and energy due to evaporation a liquid source term appears in the gaseous-phase governing equations. The liquid source terms are assigned to the gaseous phase up to a cut-off, according to a distance function which decreases exponentially with increasing distance from the centre of the droplet [21–24]. Complex chemistry is employed and the various reaction rates are computed according to the Liu et al. (2004) mechanism [20]. Validation for the implementation of the particular chemical scheme is discussed in Section 2.3 and in the Appendix.

2.2. Numerical procedure

The governing equations were solved using the three-dimensional compressible DNS code SENGA2, previously used for a variety of turbulent combustion problems [22–24,35,36]. A tenth-order explicit central difference scheme was employed for the computation of the first and second order spatial derivatives [37]. In order to enable the calculation of stiff chemistry, operator splitting between transport and chemistry was implemented. Application of operator splitting in DNS was studied and validated in previous investigations [38,39]. The transport is solved explicitly while the chemical source contribution is solved by a stiff ODE integrator. In particular, the gaseous-phase and liquid-phase transport equations were advanced using a fourth-order, low-storage explicit Runge–Kutta scheme [40] with a time step $\Delta t = 5.0 \times 10^{-9}$ s, while the implicit solver VODPK [41] was used for advancing in time the gas-phase chemical reactions. The time step was chosen to be smaller than the acoustic time scale in a grid cell ($\Delta x / \sqrt{\gamma (R/W_{air})T}$), which represents the smallest non-chemical time scale in the simulation.

2.3. Chemical mechanism

The reduced mechanism of Liu et al. (2004) [20] was used containing 22 non steady-state species and 18 global steps. The reduced mechanism was derived from a skeletal mechanism consisting of 43 species and 185 reactions. It was validated by Liu et al. (2004) [20] in terms of the ignition delay time of homogeneous heptane mixtures using the experimental data of Ciezky and Adomeit (1993) [42]. The scheme has been used previously for heptane autoignition problems [23,24,43,44] and contains methane. A parametric study was performed to examine the behaviour of the mechanism under different equivalence ratios of methane in air, pressures and temperatures considering adiabatic homogeneous n-heptane/oxidiser mixtures, with the oxidiser being a methane/air mixture (see Section 3). Homogeneous reactor calculations were also performed using the skeletal scheme [20] and are presented in Appendix A.1. In general, the ignition delay time and most reactive mixture fraction values predicted by the reduced scheme follow the same trend and only differ about 5% from the values given by the skeletal scheme. In order to examine if the mechanism employed is also representative of methane combustion, one-dimensional laminar premixed flame calculations were performed with the skeletal scheme using the Cosilab package [45] (see Appendix A.2). The laminar flame speeds and species profiles were compared with the corresponding profiles predicted by the GRI-3.0 mechanism [46] at the DNS conditions. Results are qualitatively and quantitatively similar for the two chemical mechanisms as discussed in Appendix A.2. The reduced scheme [20] was also used to