Direct numerical simulation of two-stage combustion and flame stabilisation in diesel engine-relevant conditions

Deepak Dalakoti[1], Evatt R. Hawkes[1], Marc S. Day[2], John B. Bell[2]
[1]School of Mechanical and Manufacturing Engineering, University of New South Wales, Sydney, NSW, 2052, Australia
[2]Center for Computational Sciences and Engineering, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

1 Abstract

We present preliminary results from a three-dimensional (3D) direct numerical simulation (DNS) of a spatially developing turbulent lifted flame in diesel engine-relevant thermochemical conditions with multiple step chemistry. The simulation is broadly based on the experimental flame known as Spray A, a target flame of the Engine Combustion Network. The configuration has been modified to make DNS feasible, namely we consider an equivalent gas jet with a lower Reynolds number of 15,000 but a similar global Damköhler number. The configuration consists of a round jet of n-dodecane injected into an environment with 60 bar pressure and 900 K ambient temperature, which contains 15% oxygen and 85% nitrogen by volume. The overall structure of the flame shows shows two-stage combustion and is broadly consistent with proposed conceptual models of diesel spray combustion. Low-temperature chemistry is active upstream of the high-temperature flame and persists downstream in the jet core. High-temperature chemistry occurs in the rich premixed core and in a shrouding diffusion flame. The analysis presented here focuses on the leading edge of the high-temperature flame. The leading edge is observed to be principally composed of a connected and highly convoluted structure. Upstream of this structure, ignition kernels are occasionally observed that are advected downstream and connect with the main flame. Unexpectedly, flame extinction holes are also observed, which are connected with high dissipation rates that exceed extinction limits. Flame holes are also observed to arise from flame propagation around unburned regions and upstream flame reconnection to create a hole.

2 Introduction

Flames in direct injection compression ignition (CI) engines are typically lifted from the fuel delivery nozzle. The distance from the nozzle to the flame, known as the lift-off length, is a very important parameter that determines emissions of NO_x and soot, since it controls the amount of premixing prior to combustion [19]. Even in non-autoignitive oxidiser conditions, the lifted flame stabilisation, which

Correspondence to: d.dalakoti@student.unsw.edu.au

controls the lift-off length, has been much debated [15], though the theory that now has the most support is stabilisation by the propagation of partially premixed edge-flames [8]. In CI engine conditions, the stabilisation mechanism is also very likely to be affected by autoignition phenomena, which for diesel-type fuels and typical engine conditions, occurs in the negative temperature coefficient (NTC) regime characterised by two-stage ignition [19].

A number of studies have investigated the flame structure and stabilisation mechanism in CI engine conditions. Experimental measurements in these conditions are difficult and the available data relating to the flame structure is mostly qualitative in nature. Typical measurements, e.g. [2,19,7] include OH* chemiluminiscence and/or OH planar laser-induced fluorescence (PLIF) to image high-temperature combustion zones, CH_2O PLIF to image regions undergoing low-temperature chemistry (LTC), and extinction and/or planar laser-induced incandescence PLII to image soot-containing regions. Depending on the conditions, different flame structures are observed [2, 19], but a reference condition may be taken as the spray A flame studied in the context of the Engine Combustion Network [6, 23], which has been selected to be representative of typical heavy-duty CI operating conditions with moderate exhaust gas recirculation. In this flame, a combination of the above measurement techniques, e.g. [7, 16] shows that combustion occurs in two distinct phases, with an upstream and inner region of LTC followed by a downstream, shrouding region of HTC. It is believed that the upstream/inner LTC region is a result of first-stage ignition, while the downstream HTC region is believed to consist of rich and lean premixed regions and a shrouding diffusion flame. Similar structures are also supported by numerical studies in Reynolds-averaged Navier Stokes (RANS) and large-eddy simulation (LES) frameworks [5, 22, 18, 21]. Much is not clear, however, from these studies. Most importantly, these methods do not reveal the precise reason for the flame to stabilise in the region it does.

A few major theories have been proposed to explain flame stabilisation namely: premixed flame propagation, large eddy stabilisation, edge-flame stabilisation, critical scalar dissipation stabilisation, autoignition and hybrid mode stabilisation. These theories have received varying level of support and the reader is referred to review articles [25, 15, 14]. Here we review some of the studies conducted since these reviews that are relevant to the present work.

Pei et al. [21] conducted a RANS study of Sandia Spray A [6] using transported probably density function method and suggested that the flame is stabilised by autoignition as indicated by a transport budget of the OH mass fraction; they also emphasised on the role played by turbulence on diffusion of radicals and heat out of the flame. LES of and *n*-dodecane spray in high temperature and pressure conditions was performed by Gong et al. [5]. They suggested that the stabilisation mechanism is sensitive to ambient temperature and changes from autoignition to edge-flame propagation as temperature is increased from 900 K to 1000 K. The authors also identified the presence of low-temperature chemistry upstream of the main flame, which provides radicals for the high-temperature combustion. Pei et al. [22] conducted an LES study of Spray A and found that ignition kernels form upstream of the flame base which then expand and join with the flame base; they attributed the flame stabilisation to these expanding autoignition kernels. Krisman et al. [12] performed 2D DNS of laminar dimethyl ether (DME) flame in a hot oxidiser and elevated pressure and observed the flame stabilisation mechanism to change from edge-flame propagation to autoignition with increasing oxidiser temperature and decreasing residence time. They also observed upstream high- and low- temperature chemistry branches in addition to a typical triple flame. Recently Minamoto et al. [18] performed a 3D DNS of a spatially developing jet of a partly reacted DME/air mixture issuing into an elevated ambient temperature and pressure environment and concluded that the flame is stabilised by edge-flame propagation; they also observed a pentabrachial edge-flame structure previously seen in the laminar flame study of Krisman et al. [12].

The studies discussed above are either conducted with averaged combustion models (RANS, LES), which do not reveal the full features of the flame, or (due to computational expense) are conducted at conditions not fully representative of diesel engines. With the aim to elucidate the flame structure and flame stabilisation mechanism and fill the present knowledge gap we present a three-dimensional DNS of n-dodecane jet in diesel engine conditions. Unlike the previous study by Minamoto et al. [18], the complete process of two-stage ignition is simulated in a single computation.

3 Methodology

The DNS case is set up to be broadly similar in some respects to the experimental target flame known as spray A [6]. In particular, we consider the injection of a round *n*-dodecane fuel-containing jet into a high-temperature, high-pressure quiescent ambient environment having the same thermochemical conditions as spray A. Some simplifications are necessary, however. First, given in spray A the liquid length is about half of the lift-off length, the multi-phase aspects are not expected to be particularly important to the stabilisation mechanism. As such, a purely gas phase condition is considered for the DNS. Furthermore, due to a very high Reynolds number of order of one million and a very long lifted length of order hundreds of jet diameters, DNS of the full spray A case is not anticipated to be feasible for the foreseeable future, probably beyond continuing interest in the CI engine. Therefore, the Reynolds number of the flame is considerably downscaled. The approach to setting the jet parameters is as follows. The experimentally measured centreline jet velocity, centreline mixture-fraction and jet width [6] at a location 45 mm from the nozzle are extrapolated back to a location 5 mm from the nozzle using round jet scaling laws. The Reynolds number is then reduced by a factor of 81 by reducing the jet velocity and jet diameter by a factor of nine. This approach in principle should result in a similar global Damköhler number.

In particular we consider a cubic domain (0.51*0.51*0.64 cm^3, z being the axial direction) with a round fuel-containing jet of diameter 0.17 mm at the centre. The ambient oxidiser has a temperature of 900 K, pressure of 60 bar, and contains 15% oxygen and 85% nitrogen by volume. The fuel-containing jet has a mean velocity of 28.6 m/s, a peak mixture-fraction of 0.45, and a temperature of 446 K, where the latter was determined by adiabatic mixing based on enthalpies of the oxidiser and liquid-phase fuel at 363 K (thus accounting for the fuel heat of evaporation). The inlet mean and turbulence velocity profiles were set according to a simple hyperbolic tangent profile. Inlet turbulence was generated by running a triply periodic incompressible flow, the velocity data after flow development from which was stored in a file, this is then used to interpolate velocity fluctuations for inlet turbulence to the DNS grid. The simulation considers the complete process from the beginning of fuel injection to flame stabilisation, but only the latter phase will be discussed here. A 53-species reduced chemical mechanism was used, which contains the low temperature chemical pathways [26]. Chemkin [10] was used to evaluate the reactions while EGLIB [4] was used for transport properties.

The simulation was performed using a low Mach number adaptive mesh code called LMC. Using the low Mach number approximation has the advantage of removing acoustic signals, which do not carry significant energy in the present conditions and can be safely neglected, this gives the advantage that the problem is governed by the advective Courant–Friedrichs–Lewy (CFL) number. LMC uses a second order projection method to calculate velocities, species and energy equations are integrated using spectral deferred correction (SDC) algorithm [1, 20]. The problem was solved on a 3-level dynamic adaptive grid giving an effective resolution of 2.5 micron on the edge-flame region.

4 Results

Figure 1(a) shows a 3D rendering of the flame. The flame has been cut on the X-Y quadrant to reveal the internal structure. The coloured contours are mass fraction of formaldehyde, which is generally used as marker of the low temperature chemistry [11]. The shaded white/grey surface represents mass fraction of OH, a high temperature marker. This figure shows a typical two-stage combustion structure expected at these conditions, with a cool flame upstream of the flame base and in the rich core of the jet, shrouded by a diffusion flame. This flame structure is similar to the theoretical model initially proposed by Dec et al. [2] and further elaborated by Musculus et al. [19]. Some interesting features are observed upon a close inspection of the 3D profile of OH, an example of which is shown in figure 1(c). Isolated kernels of OH (red circles) can be observed upstream of the flame base; also visible are the flame holes (blue circles) downstream of the flame base. 3D animations of the flame base show the upstream kernels are localised ignitions, a feature which has also been observed experimentally [24], which suggests that autoignition is at least partially involved in flame stabilisation. Flame holes thave not previously been observed in the present thermochemical conditions. In this study we focus our attention to the flame base, upstream flame segments and flame holes.

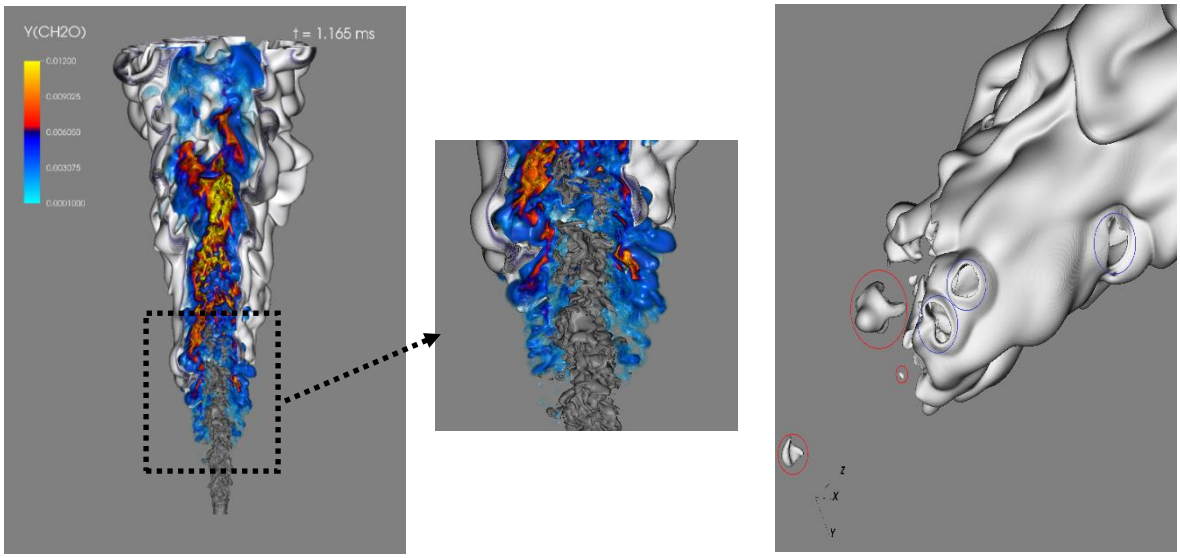

Figure 1. (a) 3D rendering of the flame. Flame has been cut in the X-Y quadrant to reveal the internal structure. Zoom of the box region is shown adjacent to the figure which shows upstream presence of formaldehyde (b) zoom view of the flame-base (c) 3D rendering of OH mass fraction. Red circles indicate upstream flame segments. Blue circles indicate flame holes.

To further understand the flame-base structure, we identify the high-temperature flame edges as the contour defined by the intersection of stoichiometric mixture fraction isosurface and the OH mass-fraction isosurface (Y_{OH}=0.0004). Figure 2 shows a time sequence of typical flame-edge axial locations versus the azimuthal angle obtained using the aforementioned definition. The flame edges are coloured by local scalar dissipation, normalised by the scalar dissipation rate corresponding to diffusion flame extinction. It is first noted that the flame base is principally composed of a connected, highly convoluted structure that extends around the entirety of the jet. This structure is visually similar to that observed in a previous DNS of a lifted flame in non-autoignitive conditions [8], suggesting that edge-flame propagation may be

important to the stabilisation mode (analysis of transport budgets and local flame speeds, not shown for brevity, confirms this). In addition to this main structure, detached segments of flame-edges are observed. For instance, the region shown in the solid black circle in frame 1 is an isolated ignition kernel that grows as it moves downstream before connecting with the main flame by frame 4. Notably the scalar dissipation rate in this kernel is quite low relative to other regions. Another kernel marked by rectangle is however not successful in surviving to main flame location, suggesting as in other studies [17, 3, 13] that scalar dissipation fluctuations are important to determining ignition probability.

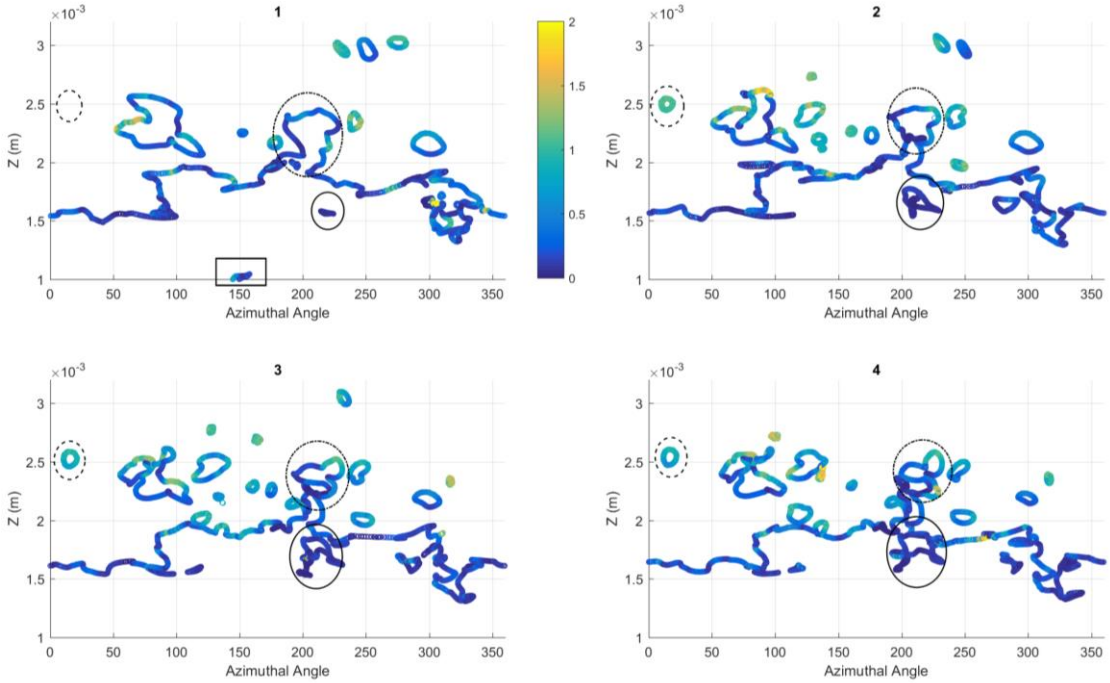

Figure 2. Axial flame base location at four time instances. The colour represents normalized scalar dissipation rate. Black ellipses encircle the expanding ignition kernel, dashed ellipses encircle expanding ignition hole and dash-dot ellipses encircle region of formation of inclusion hole.

As already noted in Fig. 1, a number of downstream flame holes are also observed. Flame holes can be produced in lifted flames by two distinct mechanisms, as first remarked by Karami et al. [8]. One of these mechanisms is via localised extinction of the diffusion flame – an example of one such region is shown in the dashed circle. Notably, this region has a high scalar dissipation rate, which leads to hole growth, similar to the situation in lifted flames in non-ignitive conditions [9]. In later times (not shown), the dissipation rate of this hole reduces and the hole disappears. This feature was not initially expected since typically the conditions that allow ignition do not favour extinction; more specifically, the critical scalar dissipation rate corresponding to non-ignition is much lower than that corresponding to diffusion flame extinction. However, scalar dissipation is a highly intermittent variable, especially at higher Reynolds numbers, and this therefore can result in dissipation rates locally exceeding the extinction dissipation rate despite the average dissipation being lower than the dissipation rate of non-ignition. Holes are not formed only by extinction, however, as shown in the region marked with the dot-dash lines. Here, a part of the main flame edge recedes downstream leaving an unburned region of the stoichiometric surface, but the flame propagates around this region and reconnects upstream, creating a flame-hole. Again, the mechanism is similar to that observed by Karami et al. [8] in the context of non-autoignitive lifted flames,

showing that some aspects of the lifted flames in these very different environments are remarkably similar.

5 Conclusions

A 3D DNS of spatially developing turbulent lifted flame was performed at diesel-engine relevant thermochemical conditions. The DNS case was set to model the experimental Sandia Spray A case. Some of the key observations of this preliminary analysis were:

- The flame presents a two-stage combustion structure with low-temperature chemistry starting upstream of the flame base and persisting downstream in richer regions in the jet core. A diffusion flame shrouds the jet.
- The flame-base is composed principally of a connected structure that is highly convoluted. It resembles similar structures observed in non-autoignitive conditions.
- In addition to the main flame, upstream isolated ignition kernels are observed. Depending on local mixing rates, some of these kernels are quenched while others survive and reconnect with the main flame.
- Flame holes were also observed. Some holes were formed by localised extinction while others formed by flame propagation around unburned regions followed by upstream reconnection.
- Overall, the results show that the flame stabilisation mechanism is quite complex. The present analysis of the high-temperature ignition appears to involve flame-propagation, autoignition, and extinction. Upstream low-temperature first-stage ignition is also probably involved. Further work on these data will seek to understand in a more quantitative way to properly characterise how these different phenomena interact and contribute to flame stabilisation.

6 References

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