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Characterisation of two-stage ignition in diesel engine-relevant thermochemical conditions using direct numerical simulation

Alex Krisman[a,b,*], Evatt R. Hawkes[b,c], Mohsen Talei[d], Ankit Bhagatwala[a], Jacqueline H. Chen[a]

[a] Combustion Research Facility, Sandia National Laboratories, Livermore, CA 96551-0969, USA
[b] School of Mechanical and Manufacturing Engineering, The University of New South Wales, Sydney, NSW 2052, Australia
[c] School of Photovoltaic and Renewable Energy Engineering, The University of New South Wales, Sydney, NSW 2052, Australia
[d] Department of Mechanical Engineering, The University of Melbourne, Melbourne, VIC 3010, Australia

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ABSTRACT

With the goal of providing a more detailed fundamental understanding of ignition processes in diesel engines, this study reports analysis of a direct numerical simulation (DNS) database. In the DNS, a pseudo turbulent mixing layer of dimethyl ether (DME) at 400 K and air at 900 K is simulated at a pressure of 40 atmospheres. At these conditions, DME exhibits a two-stage ignition and resides within the negative temperature coefficient (NTC) regime of ignition delay times, similar to diesel fuel. The analysis reveals a complex ignition process with several novel features. Autoignition occurs as a distributed, two-stage event. The high-temperature stage of ignition establishes edge flames that have a hybrid premixed/autoignition flame structure similar to that previously observed for lifted laminar flames at similar thermochemical conditions. A combustion mode analysis based on key radical species illustrates the multi-stage and multi-mode nature of the ignition process and highlights the substantial modelling challenge presented by diesel combustion.

1. Introduction

Future diesel engines will be required to attain cost-effective reductions in pollutant emissions while improving fuel economy. These improvements will arguably be easier to attain with improved fundamental understanding of diesel engine combustion, which can be built into practically useful computational models to be used in engine design. With the goal of providing this understanding, experimental and numerical studies have been carried out.

Experiments conducted in optically accessible diesel engines and chambers have visualised ignition and flame stabilisation using high speed cameras and laser diagnostics [1–3]. The results suggest that diesel combustion is a multi-stage and multi-mode process. Observations of natural chemiluminescence, soot luminosity, and planar laser-induced fluorescence (PLIF) have been able to infer the existence of low- and high-temperature autoignition, premixed combustion, and nonpremixed combustion (diffusion flames). Such visual observations form the basis for conceptual models of diesel combustion that have been proposed for conventional [1–3] and low-temperature [3] diesel engines .

In conventional diesel engines, the fuel is injected near the end of the compression stroke and the air charge is not substantially diluted with exhaust gasses. This results in highly stratified combustion with locally very rich mixtures (having high values of mixture fraction, ξ) and high temperatures. Following ignition, a quasi-stable lifted flame develops. The lifted flame is thought to exhibit a nonpremixed (diffusion flame) region, centred on the stoichiometric mixture fraction (ξ_{ST}), and a rich premixed region within the fuel jet, and, in typical ambient conditions, a region of first stage ignition (or a “cool flame”) due to low-temperature chemistry (LTC) that exists ahead of and/or inside the high-temperature chemistry (HTC) region [2–4]. The lifted flame is anchored at the most upstream location of nonpremixed combustion (the lift-off length, LOL). High levels of NOx formation are thought to occur in the hot, near-stoichiometric diffusion flame, while high levels of soot formation are thought to occur in the hot and rich inner region. Strategies to reduce pollutant formation are therefore focused on lowering peak temperatures and increasing the degree of premixing (entrainment) prior to combustion, which is closely related to parameters such as the homogeneous ignition delay time, τ, and the LOL. The reduction of pollutants therefore requires an

* Corresponding author at: Combustion Research Facility, Sandia National Laboratories, Livermore, CA 96551-0969, USA.
E-mail address: ankrism@sandia.gov (A. Krisman).

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understanding of the physical processes that govern ignition and flame stabilisation.

Autoignition in stratified mixtures at atmospheric conditions has been extensively studied (*e.g.*, see the review by Mastorakos [5]). A chief conclusion is that autoignition is sensitive to both ξ and the scalar dissipation rate, χ, such that autoignition first occurs at locations where the local mixture is near the homogeneous most reactive ξ value, ξ_{MR} [6], and the χ is low [6–13]. Experiments of autoigniting, turbulent, stratified flows at atmospheric pressure have been performed by Markides et al. [14–16]. In those studies, the configuration of an axis-symmetric fuel jet, co-flowing with hot air was considered. A statistically stationary state was achieved, whereby the rapid succession of independent autoignition events (kernels) formed at "random spots" (in physical space) and were convected downstream without establishing a connected flame surface. A direct numerical simulation (DNS) targeting similar conditions was also conducted [17], which confirmed that the kernels formed where the local mixture was near ξ_{MR} and experiencing low χ rates. Another recent experiment of a turbulent, autoigniting jet simultaneously measured ξ and temperature [18]. The results provided further experimental evidence that ignition kernels form preferably at ξ_{MR} locations where the χ is low. For diesel engine-relevant conditions, temporally and spatially resolved experimental observations of autoignition do not currently exist.

The stabilisation mode of turbulent lifted flames is an open topic of research. At atmospheric pressure, a range of stabilisation mechanisms have been proposed based on theories of, *e.g.*, premixed flame propagation [19], nonpremixed flamelet extinction [20], edge flame propagation [21–23], large scale turbulence [24], and autoignition [25–29], without a clear consensus having yet been arrived at [30,31]. For engine-relevant conditions, the stabilisation method is even less clear due to difficulties in taking well-resolved measurements. The available conceptual models [1–3] do not explicitly state which stabilisation mode or modes are responsible for diesel flame stabilisation and there remains ambiguity as to the flame structure in the vicinity of the flame base. For example, diagrams of quasi-stable diesel flames [2,3] are consistent with both flame stabilisation by two-stage autoignition and edge flame propagation into a region of first-stage autoignition (or a cool flame). A review study of stabilisation modes in diesel jets by Venugopal and Abraham [32] concluded that multiple stabilisation modes (with contradictory assumptions) could each partially explain the stabilisation behaviour observed in experiments. This indicates that the underlying physical behaviour of diesel combustion is not well understood.

A major impediment to modelling diesel combustion is the limited fidelity of experimental observation. Existing techniques are limited to qualitative descriptions of the flame structure and global observables such as LOL and τ, but additional information is required when designing and evaluating combustion models, particularly when comparing incongruous models. Additional well-resolved observations at diesel engine-relevant conditions are therefore required.

An alternative approach is to conduct DNS which serve as "numerical experiments" that fully resolve all spatial and temporal scales. The main limitation to DNS is the extreme computational cost, which is highly sensitive to the range of scales in the target simulation and the complexity of the underlying physics. Diesel combustion exhibits: multi-phase behaviour, thousands of chemical reactions, and an extremely large range of scales, which makes an engine-level application of DNS infeasible. However, by making appropriate simplifying assumptions, idealised DNS may be conducted that complement physical experiments and provide additional insight into diesel combustion. The growth of high performance computing resources has enabled several DNS investigations of diesel engine-relevant combustion at idealised conditions [33–41], the main findings of which are reviewed here.

Sreedhara and Lakshmisha [33] conducted a three-dimensional (3D) DNS study of *n*-heptane ignition in decaying isotropic turbulence. Ensemble-averaged results showed that high-temperature ignition occurred over a range of rich ξ values (approximately corresponding to ξ_{MR}) experiencing low χ. That result was consistent with prior ignition studies conducted at non-engine-relevant conditions [5].

DNS studies of the ignition of laminar [34] and turbulent [35,36] two-dimensional (2D) mixing layers were conducted by Mukhopadhyay and Abraham. The effect of mixing layer thickness (σ) on τ was studied in the laminar cases and it was observed that at low values of σ (highly stratified, corresponding to high χ values), σ and τ were negatively correlated. The turbulent ignition cases observed that both the first- and second-stages of autoignition were delayed by high values of χ [36] and the second-stage of ignition influenced the χ field due to enhanced diffusion at the leading edge of the ignition (which promoted χ) and reduced compositional gradients behind the ignition front due to heat release (which lowered χ) [35].

A DNS study of the autoignition of a sparse spray of *n*-heptane at a pressure of 24 bar was performed by Borghesi et al. [37]. The visualisation of the temperature field showed that the autoignition occurred in a "spotty" pattern. Statistics conditioned upon ξ and χ also revealed a two-staged ignition where the second-stage of ignition was negatively correlated with χ. The high-temperature ignition was also observed to occur first in mixtures slightly richer than ξ_{MR}.

Several DNS studies targeting diesel condition and using dimethyl ether (DME) fuel have recently been performed [38–41]. DME is an attractive diesel surrogate fuel as it exhibits a similar two-stage ignition and negative temperature coefficient (NTC) regime of ignition delay times also observed for diesel fuels [42]. DME is also a low-sooting, potentially renewable fuel with a high cetane number, and a potential alternative to diesel fuel in real engines [43]. DME can also be modelled with compact chemical mechanisms [44], which is attractive for DNS.

A study of laminar lifted flame stabilisation at diesel engine-relevant conditions using a 30 species reduced chemical mechanism for DME was conducted by the present authors [38]. That study considered the parametric variation of oxidiser temperature over a range which spanned the NTC regime. The study identified that hybrid edge flame/autoignition structures and stabilisation modes may exist at diesel-relevant thermochemical conditions and that a gradual transition from primarily edge flame propagation to primarily autoignition stabilisation was observed with increasing oxidiser temperature. For the case of 900 K oxidiser temperature, a main tribrachial (triple) flame was observed with an additional, fourth branch *upstream* of the stabilisation location due to LTC. The four-branched edge flame was termed a tetrabrachial flame and it broadly resembled the flame structure presented in conceptual models of conventional diesel combustion. This result suggested that a combination of both autoignition and edge flame propagation could contribute to diesel flame stabilisation.

Subsequent DNS at similar conditions by Deng et al. [39,40] also observed the hybrid flame structures and a stabilisation mode transition from edge flame propagation to autoignition with increasing oxidiser temperature for a fixed inlet velocity [39] or increasing inlet velocity for a fixed oxidiser temperature [40]. Chemical explosive mode analysis (CEMA) was used which provided further evidence in support of the findings from the previous study [38].

A 2D turbulent mixing layer DNS of ignition [41] was recently conducted by the present authors at identical thermochemical conditions to the lifted laminar flame case with an oxidiser tempera-