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A direct numerical simulation of cool-flame affected autoignition in diesel engine-relevant conditions

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Abstract

In diesel engines, combustion is initiated by a two-staged autoignition that includes both low- and high-temperature chemistry. The location and timing of both stages of autoignition are important parameters that influence the development and stabilisation of the flame. In this study, a two-dimensional direct numerical simulation (DNS) is conducted to provide a fully resolved description of ignition at diesel engine-relevant conditions. The DNS is performed at a pressure of 40 atmospheres and at an ambient temperature of 900 K using dimethyl ether (DME) as the fuel, with a 30 species reduced chemical mechanism. At these conditions, similar to diesel fuel, DME exhibits two-stage ignition. The focus of this study is on the behaviour of the low-temperature chemistry (LTC) and the way in which it influences the high-temperature ignition. The results show that the LTC develops as a "spotty" first-stage autoignition in lean regions which transitions to a diffusively supported cool-flame and then propagates up the local mixture fraction gradient towards richer regions. The cool-flame speed is much faster than can be attributed to spatial gradients in first-stage ignition delay time in homogeneous reactors. The cool-flame causes a shortening of the second-stage ignition delay times compared to a homogeneous reactor and the shortening becomes more pronounced at richer mixtures. Multiple high-temperature ignition kernels are observed over a range of rich mixtures that are much richer than the homogeneous most reactive mixture and most kernels form much earlier than suggested by the homogeneous ignition delay time of the corresponding local mixture. Overall, the results suggest

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that LTC can strongly influence both the timing and location in composition space of the high-temperature ignition.

Keywords: Autoignition; Direct numerical simulation; Cool-flame; Low temperature chemistry; Negative temperature coefficient

1. Introduction

Diesel engines play major roles in the stationary energy and transportation sectors. The technology is relatively mature and robust, however, a fine-grained understanding of the in-cylinder process, which is needed to make further advances, is currently lacking. Of particular importance are the processes of ignition and flame stabilisation, which can significantly impact both fuel economy and the formation of pollutants such as nitrogen oxides and soot.

Conceptual models of diesel combustion have been developed based on observations in optically accessible engines and chambers [1–3]. Measurements of chemiluminescence, soot luminosity, and planar laser-induced fluorescence have been used to identify regions of low-temperature chemistry (LTC) and high-temperature chemistry (HTC), and to infer the existence of combustion modes such as nonpremixed combustion, the first and second stages of autoignition, and rich or lean premixed combustion.

Musculus et al. [3] presented conceptual models for conventional and low-temperature diesel combustion. A key feature of these models was the prominence of LTC. For conventional diesel combustion, LTC is present during both the ignition and quasi-stable phases. For low-temperature diesel combustion, a quasi-stable flame does not exist and the LTC occupies a large portion of the cylinder and persists long after the high-temperature ignition develops. Experimental observations cannot resolve the smallest spatial and temporal scales, and the number and type of observables are limited.

While the conceptual models outline the overall ignition process and identify the presence of LTC, a fine-grained understanding of the LTC behaviour and its effect on high-temperature ignition is still lacking. Direct numerical simulation (DNS) can complement physical experiments by targeting idealised configurations that resolve all temporal and spatial scales. Due to the extreme computational cost of applying DNS to experimentally measured diesel spray flames, a number of simplifying assumptions are necessary. Prior DNS [4–14] have targeted diesel-relevant thermochemical conditions by neglecting: detailed chemistry [4–6], three-dimensionality [4,6–8,10,12–14], the spatial development of the jet [4,5,8,10,11], and none of these studies included realistically intense turbulence. Nonetheless, several insights have been obtained.

Sreedhara and Lakshmisha [5] considered the ignition of normal heptane in three-dimensional (3D) isotropic turbulence using a global chemistry model. Low-temperature autoignition was not discussed. They observed that high-temperature autoignition occurred in rich mixtures with low scalar dissipation rates (χ). This was consistent with previous DNS at non-diesel-relevant conditions which identified that autoignition occurs near a most-reactive mixture fraction value ξ_{MR} [15] conditioned upon χ [15,16].

Mukhopadhyay and Abraham conducted two-dimensional (2D) DNS of ignition for laminar [8] and turbulent [10] mixing layers at diesel-relevant conditions. A two-stage autoignition process was observed such that the first stage of autoignition was not sensitive to χ but the second stage of autoignition was delayed for high scalar dissipation rates [8]. For the turbulent case, both stages of autoignition occurred first at regions with low χ [10].

A DNS of lifted, laminar flame stabilisation with a reduced dimethyl ether (DME) chemistry by the present authors [12] identified several novel combustion features. Edge-flame, or hybrid edge-flame/autoignition structures were observed at diesel-relevant conditions. These flames resemble classic tribrachial (triple) flames with leading rich and lean premixed branches converging to a trailing nonpremixed branch at a triple-point. However, additional branches *upstream* of the triple-point were observed that are due to either the first (LTC) or second (HTC) stages of autoignition. In particular, for the case where the oxidiser temperature was 900 K, a single upstream branch was observed due to LTC. This branch was initiated at a mixture fraction, $\xi_{MR,1}$, corresponding to the shortest first-stage ignition delay time, τ_1, as calculated in a homogeneous reactor. A transport budget analysis [17] of the LTC branch revealed a transition from a convection-reaction balance to a diffusion-reaction balance. This suggested that the LTC branch transitioned from an autoignition to a diffusive "cool-flame". The LTC branch merged with the main tribrachial flame further downstream, producing a four-branched or tetrabrachial flame that is

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