



Full Length Article

A comparison of high-temperature reaction and soot processes of conventional diesel and methyl decanoate



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ABSTRACT

This paper aims to improve a knowledge base of methyl decanoate, a long alkyl-chain biodiesel surrogate fuel gaining popularity in engine combustion research. To this end, a comparative study on diesel and methyl decanoate combustion has been conducted with a focus on high temperature flame structures and soot distributions in an optically accessible single-cylinder light-duty common-rail diesel engine. The in-cylinder pressure trace and apparent heat release rate curves were well matched for both fuels when the same amount of fuel energy was supplied, which confirmed very similar combustion phasing. Planar laser induced fluorescence of hydroxyl radicals (OH-PLIF) and planar laser induced incandescence (PLII) as well as line-of-sight integrated chemiluminescence imaging of cool-flame signals and electronically excited OH (OH*) were performed for various crank angles to capture the temporal and spatial development of diesel and methyl decanoate flames. The results show that both the cool-flame and OH radical signals are higher during methyl decanoate combustion with their wider distributions and larger in-cylinder volume fraction when compared to that of diesel, suggesting enhanced low- and high-temperature reactions due to oxygen in fuel. The oxygenated methyl decanoate with no aromatics in its molecular structure shows a lower soot formation rate than diesel as evidenced by delayed appearance of LII signals and lower overall intensity. This difference is significant even if the lower sooting propensity of methyl decanoate and thus less attenuation in the laser beam is considered. The rate of soot oxidation is also higher for methyl decanoate not only due to oxygen in fuel but also higher OH radicals surrounding smaller soot pockets compared to diesel.

1. Introduction

With reserves for crude oil running low and the increasing price of petroleum diesel, biodiesel made from naturally occurring resources such as vegetable oils and animal fats [1–8] has been considered as an alternative diesel fuel [5–7,9]. In contrast to conventional biodiesel fuels from food-crop-based feed stocks, next generation biodiesel fuels can be produced in large amounts from dedicated energy crops and micro-algae [1–6,10–12]. These feed stocks are domestic resources and therefore help reduce the dependence on the volatile global oil market. This diversification, however, presents a challenge for the control of biodiesel combustion, which requires extensive tests before it is used in engines.

Various engine performance and emissions testing has been performed for biodiesel fuels in pure and blended formulations, with the majority of these studies reporting a reduction in engine-out emissions of particulate matters but an increase in oxides of nitrogen (NO_x) and fuel consumption [5,13–15]. These emission trends are the result of

complex interactions between physical and chemical processes occurring inside the cylinder of the engine. Biodiesel has significantly different physical properties compared to diesel, including a higher boiling-point temperature, viscosity and density [5,13]. In addition, it has a significantly different chemical structure – notably, biodiesel is an oxygenated fuel, affecting air–fuel mixing stoichiometry [16–19] as well as chemical kinetics and pollutant formation [16,17,19,20]. Even between different biodiesel fuels there are significant variations in molecular structure which impact engine performance and emissions. For example, depending on the type of algae, fuels with 10 to 20 atoms in the carbon chain can be produced, with varying degrees of unsaturation (i.e. double bonds in alkyl chains) [6,7,13,21]. Folding in the increased diversity of feedstock, there is a clear need for enhanced understanding of biodiesel combustion fundamentals.

Conventional biodiesel is a multi-component fuel composed of various fatty acid methyl esters (FAME) such as methyl palmitate (C₁₇H₃₄O₂), methyl stearate (C₁₉H₃₆O₂), methyl oleate (C₁₉H₃₆O₂), methyl linoleate (C₁₉H₃₂O₂) and methyl linolenate (C₁₉H₃₀O₂) [22–24].

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Due to the variety and complexity of the molecular structure of biodiesel, research on the mechanics of its combustion chemistry is challenging and developing a representative model for biodiesel is difficult and expensive to accomplish. Furthermore, conducting combustion experiments using long chain (*i.e.* high molecular weight) FAME is challenging due to difficult vaporisation. To simplify this task, it is common practice to use a surrogate fuel with a simpler, more defined molecular structure for studies in biodiesel combustion. This approach helps reduce the size of chemical kinetic reactions, while still representing the role of the molecular structure in biodiesel combustion. For example, previous research has proposed methyl butanoate ($C_4H_8O_2$) as a suitable surrogate fuel for biodiesel due to its simple molecular structure [9,22]. However, the low molecular mass and small carbon chain of methyl butanoate, coupled with a lack of observed negative temperature coefficient (NTC) behaviour from previous research [24–26], imply that methyl butanoate is not as suitable as a biodiesel surrogate fuel as previously hypothesised. Methyl decanoate ($C_{11}H_{22}O_2$) is another biodiesel surrogate fuel gaining popularity. The longer carbon chain (*i.e.* alkyl carbon chain of 10 single bonds) provides a better representation of biodiesel in terms of molecular structure and mass [25] while reports of the ignition delay and negative temperature coefficient (NTC) behaviour are similar to conventional biodiesel fuels [24,27,28]. Furthermore, engine-out emissions from methyl decanoate have been reported to closely follow that of soybean derived biodiesel [29]. Optical diagnostics also confirmed low sooting properties of methyl decanoate compared to ultra-low sulphur diesel [30] while the overall flame structures of two fuels characterised by a wall-interacting jet are very similar [31]. Importantly, the detailed chemical kinetics mechanisms are available in the literature [22,23,26,32], which further justifies the use of methyl decanoate as a biodiesel surrogate fuel in engine combustion research.

Despite these benefits, little is known about the in-cylinder development of flames and soot in an automotive diesel engine. Previous studies conducted in a constant volume combustion chamber [17] and a large-bore, heavy-duty diesel engine [30] cannot reproduce the

significant geometry and flow effects in a small-bore diesel engine. This study bridges that gap by performing planar laser induced fluorescence of hydroxyl (OH-PLIF) and planar laser induced incandescence (PLII) as well as line-of-sight integrated imaging of cool-flame chemiluminescence and electronically excited hydroxyl radicals (OH^*) in an optically accessible single-cylinder light-duty diesel engine. The comparison of these signals allows for the study of the relationships between different combustion species and how they interact within the piston bowl. In the same engine and at fixed operating conditions, the same diagnostics are repeated for a conventional diesel fuel, achieving the direct comparison of flame structures and soot distributions.

2. Experimental setup and diagnostics

2.1. Engine setup and operating conditions

The experiments were performed using a single cylinder light-duty optical diesel engine as shown in Fig. 1. A summary of the engine specifications and operating conditions is found in Table 1. The engine has a 497.5 cm^3 displacement volume with a bore of 83 mm, a stroke of 92 mm and a compression ratio of 15.5. Optical access is made possible by a quartz window located on the top of the extended piston in which, through the use of a 45° mirror located in a hollowed out section of the piston body, can allow for a camera to be positioned to capture the events occurring within the combustion chamber. Part of the cylinder liner is also made of quartz which allows for laser access to perform imaging diagnostics. To prevent the piston bowl rim from obstructing the input laser crank angles ($^\circ\text{CA}$) close to top dead centre (TDC), a 35-mm wide portion of the piston bowl rim was removed as illustrated in Fig. 1. Previous studies confirmed that this bowl-rim cut-out does not impact the bulk-gas flow structures [33,34] and the flame development during the main combustion event, which completes before the flames reach the cut-out region [31,35–37]. The engine was motored at 1200 RPM with an AC motor connected to the high-inertia flywheel on the crank case. Throughout the experiments, a water heater/circulator was

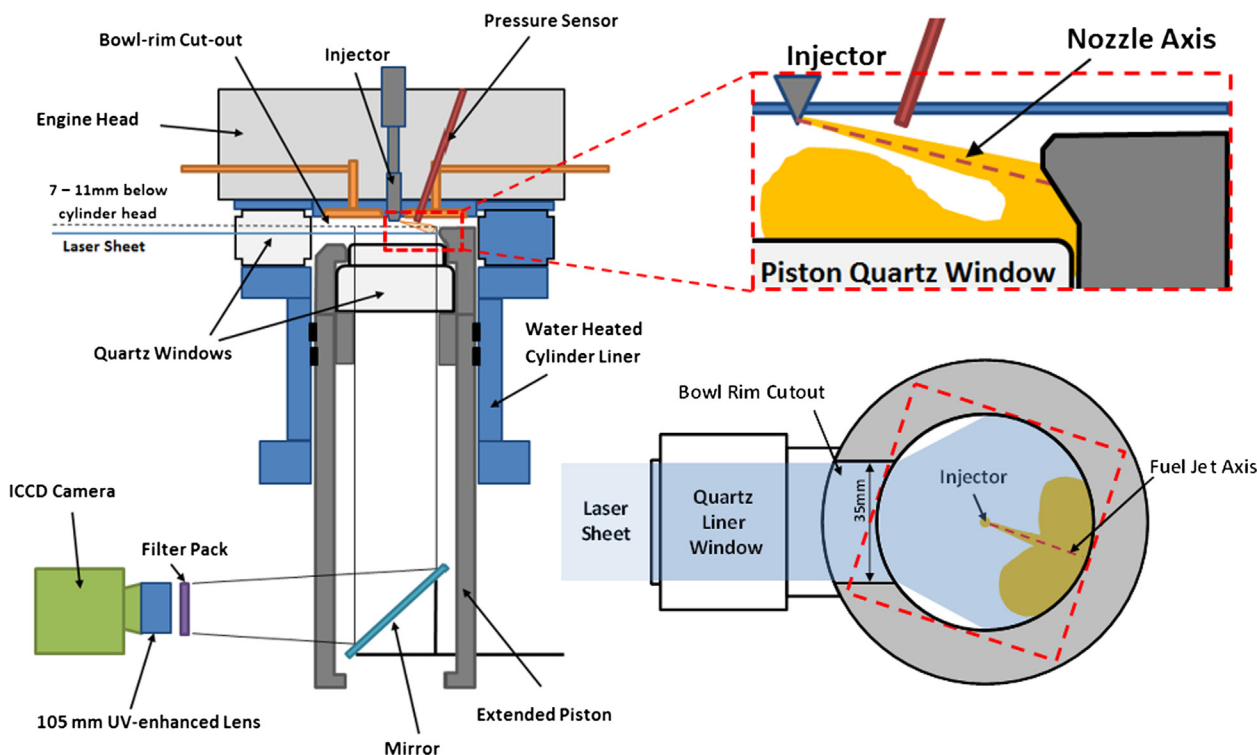


Fig. 1. Engine schematic (left), a close up of the wall-interacting fuel jet (top right), and the top view of the wall-interacting jet orientation with the input laser sheet (bottom right).

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