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Effects of the direct-injected fuel's physical and chemical properties on dual-fuel combustion

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HIGHLIGHTS

- Distillation curve impact was studied on dual-fuel combustion.
- Cetane number is not sufficient to fully describe the fuel's chemical kinetic behavior for all conditions.
- A fuel's distillation curve has a minimal impact in combustion characteristics.
- Differences in combustion characteristics stem from NTC region at low equivalence ratios.

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ABSTRACT

An experimental and computational study was conducted to explore the effects of the physical properties of the high reactivity fuel in a Reactivity Controlled Compression Ignition (RCCI) combustion dual-fuel strategy. The objective is to systematically isolate the effects of the boiling characteristics of the direct injected fuel in dual-fuel combustion strategies with different levels of fuel stratification. In all studies, iso-octane was used as the low reactivity fuel. The effect of high reactivity fuel physical properties was investigated by comparing the results of engine experiments using two fuels with equal cetane numbers (CN), but different boiling characteristics. The two fuels are 1) a certification grade Ultra Low Sulfur Diesel (ULSD) fuel with a cetane number of 45 and 2) a blend of 21% iso-octane and 89% *n*-heptane with a cetane number of 45. Computational fluid dynamics (CFD) modeling using the KIVA-3v code with a discrete multi-component evaporation model capable of capturing important physical property influences and a multi-fuel chemistry model capable of describing the chemical kinetics of single and multi-component fuels was used to explain the observed differences in the experiments. It was found that the different boiling curves of the two fuels have minimal effect on the combustion phasing at early and late injection timings. Differences in the combustion phasing were explained by differences in the chemical characteristics of each fuel that could not be matched solely by fixing the CN.

1. Introduction

In recent years, a lot of attention has been devoted to highly premixed, low temperature combustion strategies that have the potential to achieve high efficiency and ultra-low NOx and soot emissions [1–7]. Although promising, controlling combustion phasing and duration is a challenge. Reactivity Controlled Compression Ignition (RCCI) combustion accomplishes combustion phasing and duration control by using two different fuels that have different reactivity profiles, one has a high reactivity and the other a low reactivity [8–16]. By premixing the low reactivity fuel and direct-injecting the high reactivity fuel later in the cycle, a gradient of ignition delay is created. The resulting ignition process is staged, where the regions with more high reactivity fuel ignite first and

Abbreviations: ATDC, after top dead center; CA, crank angle; CA10, crank angle of 10% mass fraction burned; CA50, crank angle of 50% mass fraction burned; CN, cetane number; DI, direct injected; DISOI, direct injection start of injection; DOI, duration of injection; EGR, exhaust gas recirculation; EOC, end of combustion; ESU, expansion stroke utilization; FACE, fuels for advanced combustion engines; FTIR, fourier transform infrared; GCR, group chemistry representation; GIE, gross indicated efficiency; HCC, homogeneous charge compression ignition; HRR, heat release rate; IMEP, indicated mean effective pressure; LTC, low temperature combustion; LTHR, low temperature heat release; MFB, mass fraction burned; NTC, negative temperature coefficient; PLIF, planar laser induced fluorescence; PRF, primary reference fuel; RCCI, Reactivity Controlled Compression Ignition; SOC, start of combustion; TDC, top dead center; ULSD, ultra low sulfur diesel.

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the other regions ignite in sequence depending on the local ignition delay. This staged ignition process leads to a more gradual increase of the cylinder pressure than a fully homogenous charge and the choice of injection timing and the ratio between the two fuels can be used to tailor the duration of combustion and the start-of-ignition, respectively.

The high reactivity fuel of choice for most of the previous RCCI work has been diesel fuel. To avoid the complications of carrying two fuels, Splitter et al. [17] proposed a "single fuel" RCCI strategy where gasoline doped with a cetane improving additive (2-EHN) was used as the high reactivity fuel, as an alternative to diesel fuel. Many other types of fuels with high reactivity characteristics can potentially be used to stratify the mixture and potentially improve the combustion process. Since these fuels may have different physical and chemical characteristics over a range of temperatures, it is of interest to understand the impact of these properties on the resulting combustion event. The present study focuses on the effects of the distillation curve (i.e. the physical properties) of the direct-injected fuel on the combustion process under RCCI and premixed substitution combustion regimes. The objective of this work is to systematically isolate the effects of the boiling characteristics of the direct injected fuel in dual-fuel combustion strategies with different levels of fuel stratification. Such a fundamental understanding of the physical property effects on dual-fuel combustion is not clear from current literature. The current work will quantify the effects of the boiling characteristics in a general way that will help guide future work on fuel research for advanced combustion strategies. Two different direct-injected fuels with different physical properties, but the same cetane number were experimentally tested. Detailed non-reacting Computational Fluid Dynamics (CFD) modeling and static homogeneous ignition delay calculations were then used to help interpret the results and evaluate the relative importance of physical and chemical property effects under RCCI combustion conditions.

2. Materials and methods

2.1. Experimental setup

The engine used for the experiments is a Caterpillar C15 single-cylinder engine. Table 1 shows the engine specifications and Fig. 1 shows a schematic of the laboratory setup. All gaseous emissions were analyzed with a Thermo-Fischer fourier transform infrared (FTIR) analyzer and smoke was measured with an AVL 415S smoke meter. A turbocharger is simulated by pressurizing a closely-coupled intake surge tank with compressed air. The original direct injection fuel system has been replaced by the one specified in Table 2. A port-fuel-injection system was installed to provide the premixed fuel.

Table 1
Single-cylinder test engine specifications.

Displacement	2.44
Bore [mm]	137.2
Stroke [mm]	171
Con. Rod Length [mm]	270.6
Number of Valves	4
IVC [°ATDC]	−154
EVO [°ATDC]	113
Swirl Ratio	0.7
Piston Type	Articulated
Piston Profile	Stock Bowl
Compression Ratio	16.9:1 (stock)

2.2. Fuels

The direct-injected fuels chosen for this experiment were a 2007 certification diesel fuel with a cetane number of 45 and a blend of 21% iso-octane and 79% *n*-heptane (i.e., PRF21) with a cetane number of 45. The fuels' properties are summarized in Table 3. These fuels have the same cetane number, but significantly different physical properties [18]. Fig. 2 shows the distillation curves of diesel fuel and PRF21 and highlights the differences in the boiling characteristics of the two fuels. 100 ppm of Infineum R655 lubricity improver was added to the PRF21. The lubricity improver has been found to have a minimal impact on the ignition characteristics of the fuels. The premixed fuel used for all experiments and simulations was neat iso-octane.

2.3. Operating conditions

For all tests, the engine was operated at 1300 rev/min, a typical speed of operation for the engine used in the experiments at chosen load conditions. A single, direct-injection of either diesel fuel or PRF21 was used with a constant rail pressure of 500 bar. The rail pressure was chosen as a typical value for RCCI operation in order to avoid excessive fuel penetration and wall wetting. Additionally it also allows longer injection durations in order to achieve sufficiently stratified, stable RCCI operating conditions across the whole range of injection timings. The direct-injection timing was varied from 140° before top dead center (BTDC) to 15° BTDC to target operation in the fully premixed regime, the partially stratified RCCI regime, where combustion is kinetically controlled, and the highly stratified regime, where mixing effects are more important.

Two different equivalence ratios were tested and varied by changing the intake air pressure while maintaining the intake air temperature constant. No exhaust gas recirculation (EGR) was used. The total fuel energy per cycle was kept constant at 3200J for all comparisons. The premixed ratio (i.e., energy percentage of iC_8H_{18}) was held constant at 80% by energy for most of the experiments. The premixed ratio of 80% was chosen in order to allow stable and safe operation of the engine across the whole range of start of injection (SOI) timings for both equivalence ratios tested. A higher premixed ratio of 95% was tested to verify the effects of the direct-injected (DI) fuel quantity at the lowest equivalence ratio. The base conditions for the experiments are summarized in Table 4.

2.4. Computational model

Computational modeling was performed using an in-house computational fluid dynamics (CFD) code based on the KIVA family of codes. The code includes improved physical models developed at the University of Wisconsin's Engine Research Center (ERC) [19]. The spray model for this study uses the Lagrangian-Drop and Eulerian-Fluid (LDEF) approach. In order to reduce the grid size dependency of the LDEF spray model and allow accurate spray simulation, the Gasjet model of Abani et al. [20] is used to model the relative velocity between the droplets and gas phase in the near nozzle region. The Kelvin Helmholtz-Rayleigh Taylor (KH-RT) model was used to model the spray break-up [21]. The Re-Normalization Group (RNG) k-ε model was used for the turbulent flow calculation [22]. The droplet collision model is based on O'Rourke's model and was expanded by Munnanur [23] to include a more complete list of collision outcomes that considers effects of bounce, coalescence, fragmenting and non-fragmenting separations. A wall film sub-model was used to model droplet interaction with the wall [24]. The physical properties of the fuel are modelled using a multi-component evaporation model [25] that is able to capture the distillation curve of diesel fuel. For HCCI validation

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