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Investigation of the LTC fuel performance index for oxygenated reference fuel blends

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HIGHLIGHTS

- We describe a previously introduced new fuel performance metric for LTC engines.
- Driving cycle simulations provide real-world engine operating conditions.
- We modeled HCCI engines to determine fuel operating envelopes.
- We calculated the LTC performance index for oxygenated reference fuels mixtures.
- The LTC fuel performance index is not well-correlated to octane number.

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ABSTRACT

A new metric for ranking the suitability of fuels in LTC engines was recently introduced, based on the fraction of potential fuel savings achieved in the FTP-75 light-duty vehicle driving cycle. In the current study, this LTC fuel performance index was calculated computationally and analyzed for a number of fuel blends comprised of *n*-heptane, isooctane, toluene, and ethanol in various combinations and ratios corresponding to octane numbers from 0 to 100. In order to calculate the LTC index for each fuel, computational driving cycle simulations were first performed using a typical light-duty passenger vehicle, providing pairs of engine speed and load points. Separately, for each fuel blend considered, single-zone naturally aspirated HCCI engine simulations with a compression ratio of 9.5 were performed in order to determine the operating envelopes. These results were combined to determine the varying improvement in fuel economy offered by fuels, forming the basis for the LTC fuel index. The resulting fuel performance indices ranged from 36.4 for neat *n*-heptane (PRF0) to 9.20 for a three-component blend of *n*-heptane, isooctane, and ethanol (ERF1). For the chosen engine and chosen conditions, in general lower-octane fuels performed better, resulting in higher LTC fuel index values; however, the fuel performance index correlated poorly with octane rating for less-reactive, higher-octane fuels.

1. Introduction

Low-temperature combustion (LTC) strategies offer the potential of improved fuel economy and reduced pollutant emissions, both necessary to meet the increasing demands of federal regulations. Although LTC concepts such as homogeneous charge compression ignition (HCCI) engines have received significant research attention since first introduced [1,2]—and continue to receive attention, albeit alongside related concepts such as reactivity controlled compression ignition (RCCI) [3–6] that varies fuel reactivity by stratifying a lower reactivity fuel like gasoline with a highly reactive fuel like diesel—a number of research challenges remain. In particular, unlike spark-ignition (SI) and compression-ignition (CI) engines where the spark and fuel injection initiate combustion, respectively, in HCCI and related engine concepts complex autoignition chemistry controls combustion timing. As a result, since the fuel chemistry plays a stronger role, varying fuel composition can result in a significantly different and potentially smaller range of operation in HCCI engines. In addition, while the lower combustion temperatures of HCCI combustion offers reduced nitrogen oxide (NO_x) emissions, it also results in high levels of carbon monoxide and unburned hydrocarbons [7]. Yao et al. [7] reviewed these and additional challenges in HCCI engine

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research, and the various strategies under investigation to solve them.

Early studies on HCCI strategies with gasoline [1,2,8] found that successful HCCI combustion could only be achieved in limited operating ranges. With a typical SI compression ratio, at low loads and while idling the knock resistance of typical high-octane gasoline prevents the initiation of autoignition; on the other hand, knocking can occur at higher loads. Diesel fuel, on the other hand, is much more reactive than gasoline and ignites too early when used in a premixed charge at the high compression ratios typical of CI engines [9]. While strategies to use typical gasoline and diesel fuels in HCCI engines have been investigated [7,9], another option is to find new fuels or fuel blends that may offer more attractive performance. Various groups studied the operating ranges of different fuels in HCCI engines with the goal of identifying attractive species or mixtures [10–23]. The fuels studied include—but are not limited to—real fuels such as gasoline [10,11,17,20–22], diesel [10,18,20], and Jet B [18]. In addition, numerous studies focused on neat fuels and mixtures of such, including *n*-butane [11], neat and blends of the primary reference fuels (PRFs) *n*-heptane and isooctane [10–13,16,17,19,22,23], and mixtures of the PRFs with toluene [22,23] and ethanol [17,22,23] both individually and together [23]. Other groups investigated the behavior of alcohols in HCCI engines, including neat butanol [20] and ethanol [24–26,20]; wet ethanol also received significant attention as a neat fuel due to the potential for increased overall energy efficiency by avoiding or reducing distillation and dehydration [27–29]. The low reactivity of alcohols such as ethanol and methanol motivated additional research into operating HCCI engines using blends with more reactive fuels/additives such as *n*-heptane [30], diethyl ether [31,32], dimethyl ether [33–36], and di-tertiary butyl peroxide [37]. In the opposite direction, other efforts studied injecting water into the engine cylinder to temper the reactivity of highly reactive fuels [33,38–41]. However, nearly all of these efforts focused on a small subset of fuels and a narrow range of operating conditions; furthermore, a robust method to rank—and potentially predict—fuel performance in HCCI and other LTC-strategy engines has not yet emerged.

The octane rating, typically given by the research octane number (RON) and/or motor octane number (MON), is used to rank the resistance to knock of a gasoline-like fuel in SI engines, where a higher number indicates greater knock resistance. These values are determined by comparing the knocking characteristics under standardized conditions to those of a binary mixture of the PRFs *n*-heptane and 2,2,4-trimethylpentane (isooctane), where 0 and 100 correspond to the volume percentage of *n*-heptane and isooctane, respectively. However, various studies showed that octane rating does not adequately predict autoignition in HCCI engines [14,15,22,23], due to the fact that real fuels consist of more complex mixtures of fuel components compared to the PRFs.

A number of new metrics have been proposed to better quantify fuel performance in HCCI engines. Kalghatgi [14] first introduced the octane index, which combines the RON and MON values for a fuel with an empirical parameter related to engine-specific operating conditions. Later, Shibata and Urushihara [15] developed three HCCI fuel indices, including the relative HCCI index that combines MON with information about the fuel composition. However, as Rapp et al. [22] recently showed in a study of the performance of various fuels in a Cooperative Fuel Research (CFR) engine operating in HCCI mode, neither of the octane or relative HCCI indices can predict the autoignition behavior for a wide range of fuels. In particular, the correlations for both indices poorly predict the behavior of gasoline blends with naphthenes, aromatics, and ethanol. Truedsson et al. [23] recently presented another number for specifying fuel performance in HCCI engines: the Lund–Chevron HCCI Number, based on the required compression ratio for autoignition at a particular combustion phasing.

However, while the various existing indices partially succeed in describing the combustion behavior of gasoline-like fuels in HCCI engines, none relate the fuel performance to fuel savings in realistic engine conditions. This motivates the development of a new metric for measuring the performance of fuels in LTC engines in order to both rank fuels and predict future performance. Such a metric could also be used to identify attractive fuels for HCCI engine operation or assist in the development of new fuels. Niemeyer et al. [42] recently introduced a novel LTC fuel index that combines information about the fuel operating envelope—the feasible engine speeds and loads for a fuel in HCCI mode—with the operating conditions needed under realistic engine operation. As such, this LTC index ranks poorly fuels with wide operating ranges that are outside the conditions needed for typical vehicles in typical driving conditions, because using such a fuel in an HCCI engine would have a minimal impact on overall fuel consumption.

By gauging the impact of various fuels on real-world fuel economy via transient driving cycles, the current approach is distinct from the (significant) prior efforts focused on advanced internal combustion engine development. However, certain studies summarized here used transient driving cycles to predict fuel economy and emissions improvements using advanced engine modes such as HCCI and related concepts. Zhao et al. [43] simulated a hybrid SI/HCCI gasoline engine through the European New Emission Drive Cycle, although they reported achieving only moderate improvements in fuel economy and emissions due to the limited range of operating conditions in HCCI mode. Curran et al. [44] used five steady-state modal points [45,46] to approximate the EPA Federal Test Procedure (FTP-75) driving cycle, then compared fuel economy and emissions of RCCI, diesel HCCI, and conventional diesel combustion by performing engine experiments over the set of conditions. Similarly, Ortiz-Soto et al. [47] developed an engine and vehicle modeling framework that they used to simulate a hybrid SI/HCCI engine-powered vehicle over the EPA UDDS, Highway Fuel Economy Test, and US06 driving cycles. Using similar methodologies to the above efforts, Gao et al. [48] and Ahn et al. [49] modeled hybrid-electric vehicles capable of conventional/HCCI operation. Both studies found that while conventional vehicles benefit from HCCI operation in terms of fuel consumption and emissions, HCCI offered little improvement to hybrid-electric vehicles due to its limited operation range in the higher loads where the electric motor was not needed. Unlike the current work, the studies cited here studied the performance of typical gasoline fuels over the driving cycles, rather than exploring the performance of various fuels or seeking to find new fuels that might offer wider HCCI operating envelopes.

The current study builds on an earlier effort [42] that introduced a new LTC fuel performance index by determining the indices for a number of fuel blends comprised of *n*-heptane, isooctane, toluene, and ethanol in various combinations and ratios. The range of fuels investigated here is similar to that studied by Truedsson et al. [23,50–52] in their experiments on the compression ratio required for autoignition; however, unlike the current computational approach those experiments held equivalence ratio and engine speed constant. Following the general procedure first introduced by Niemeyer et al. [42], we performed driving cycle simulations for a typical light-duty passenger vehicle to generate steady-state operating points in terms of engine speed and torque, and also obtained the corresponding baseline SI engine fuel consumption for these operating points. Next, HCCI engine simulations were performed for a variety of fuel blends in order to determine their operating ranges. The resulting operating envelopes were combined with the necessary operating points for the driving cycle, and we then calculated the LTC fuel index for each blend studied by